Simulator Development for Nanoelectronic and Electromagnetic Devices

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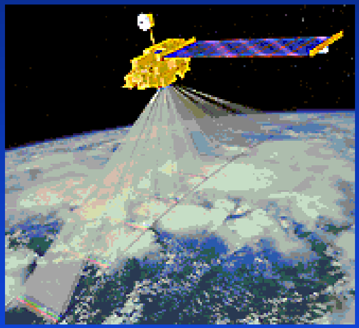
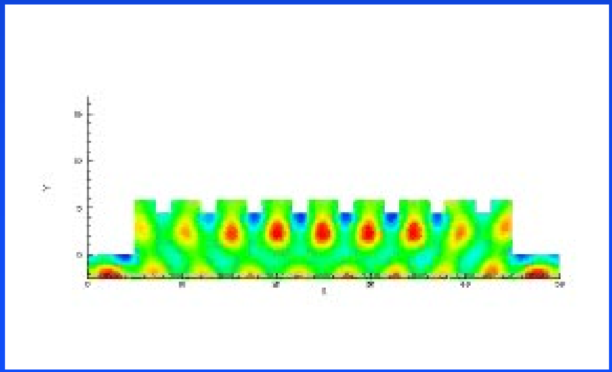
High Performance Computing at JPL

- JPL is the Lead Center for Robotic Space Exploration
  - Deep Space Missions
  - Earth Observing Missions
- JPL Builds Observational Systems for Remote Sensing
  - Imaging instruments across all wavelengths
  - Spectroscopic and in-situ instruments for planetary investigation
  - Fundamental technology development for new instruments
- JPL High Performance Computing is a Key Technology
  - Modeling and simulation of devices and instruments
  - Rapid data reduction and analysis
  - Advanced software design, implementation and application

http://mars.jpl.nasa.gov



http://www-misr.jpl.nasa.gov



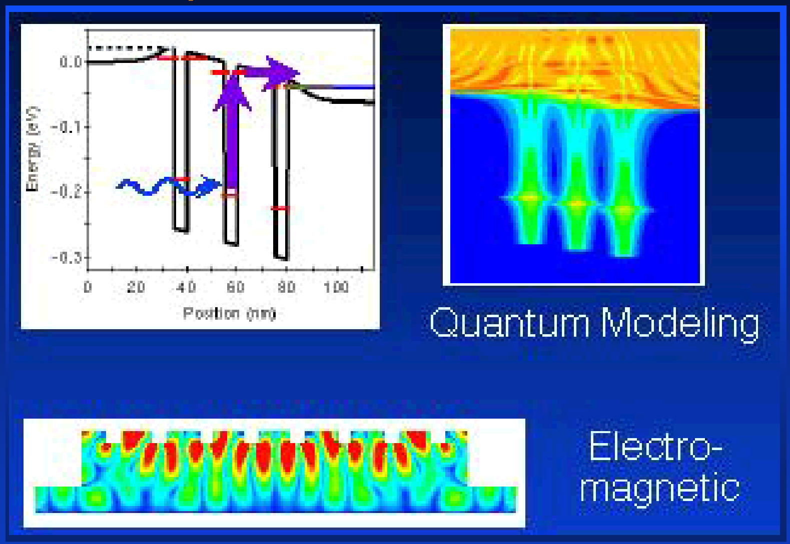
High Performance Computing at JPL

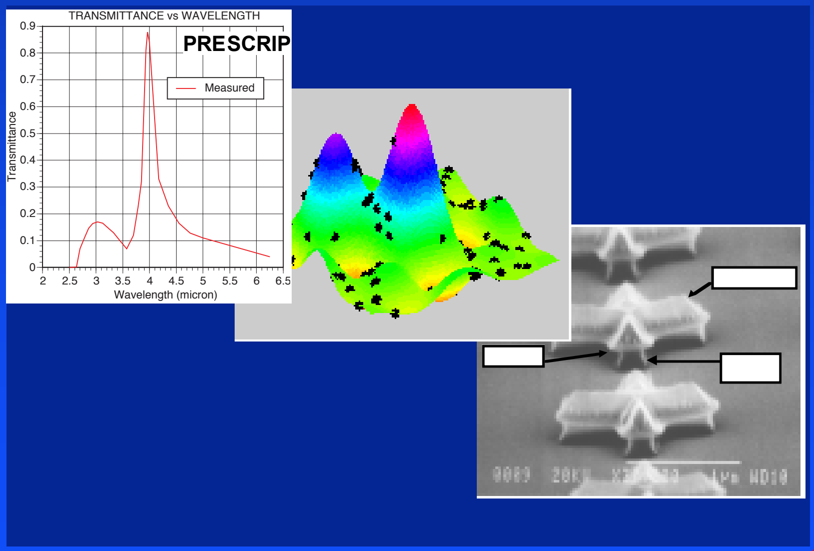
Current Work (Selected)

- **Computational** Modeling and Design

  Through the application of high performance computing, achieve physics-based, high-fidelity modeling of components needed for JPL missions

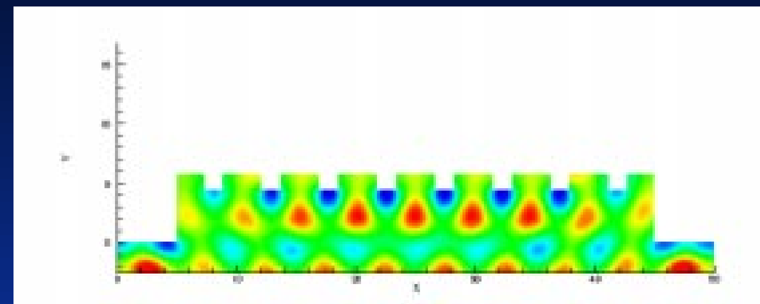
  - Electronic Modeling of Nanoelectronic Devices
  - Electromagnetic Modeling of Microelectronic Devices



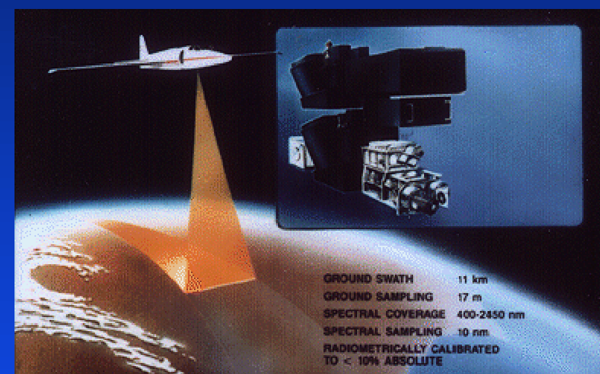


High Performance Computing at JPL
Current Applications (selected)

- Advanced Electromagnetic Design
  - Designed grating structures to optimize light coupling into quantum well infrared photodetectors; performance enhanced a factor of 10 for imaging arrays.

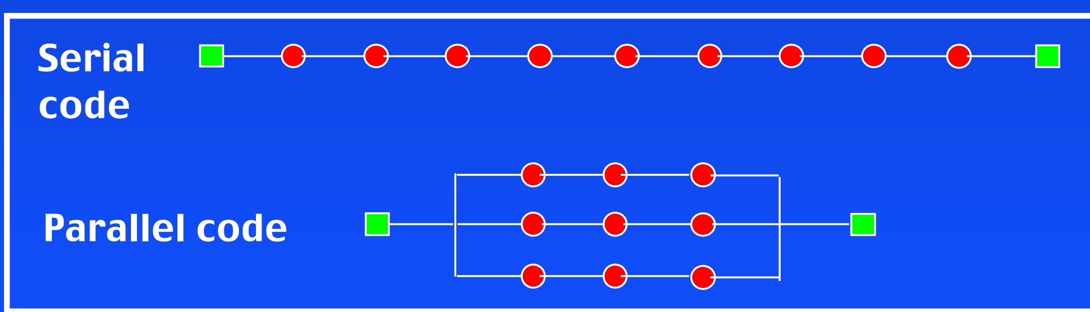


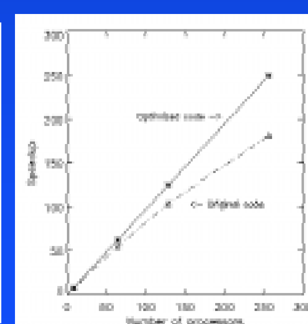
- Rapid Data Reduction and Analysis
  - Software for atmospheric retrieval (removing effects of atmospheric scattering from measured data) moved to advanced parallel computers. Used in Airborne Visible InfraRed Imaging Spectrometer (AVIRIS) flight project.

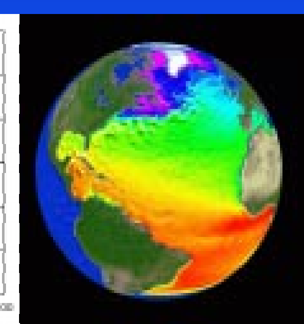


http://makalu.jpl.nasa.gov/aviris.html

- Code Optimization and Parallelization
  - We maintain expertise in application software development for large parallel computing platforms.



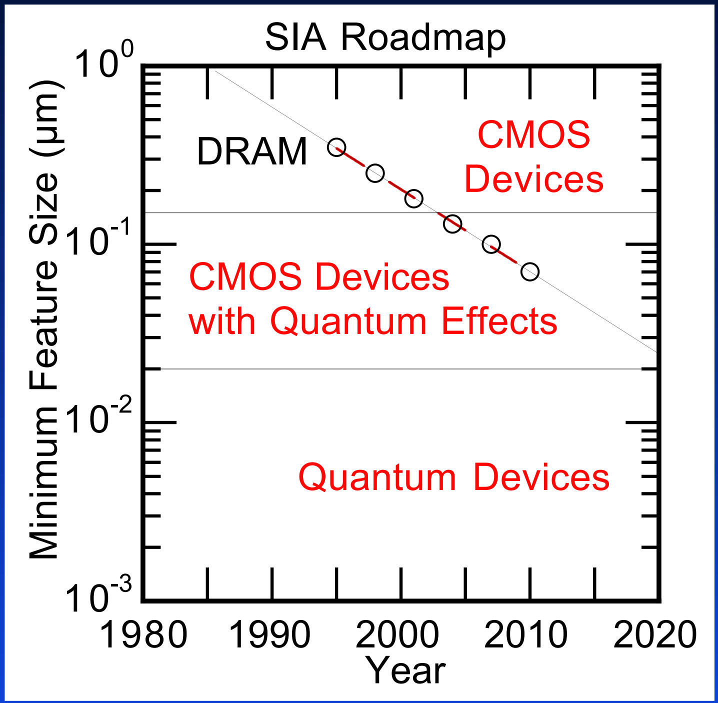


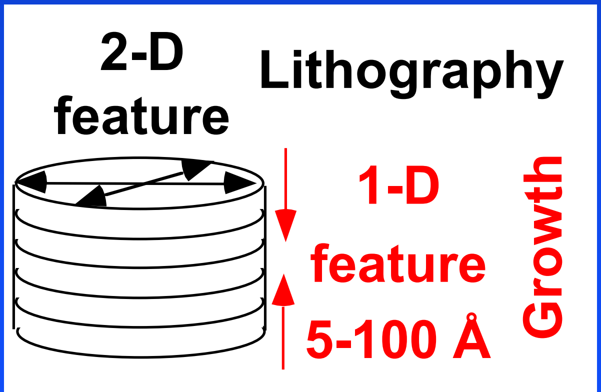


Simulator Development for Nanoelectronic and Electromagnetic Devices

- **Motivation**
- **1D modeling**
  - Bandstructure
  - Resonant Tunneling
  - NEMO (NanoElectronic MOdeling)
- **3D modeling**
  - Quantum Dots
  - NEMO-3D
- **Design and Synthesis**
  - GENES (Genetically Engineered Nanostructured Devices)
- **Future Efforts**
- **Conclusions**

Microdevices Head for Atomic Dimensions



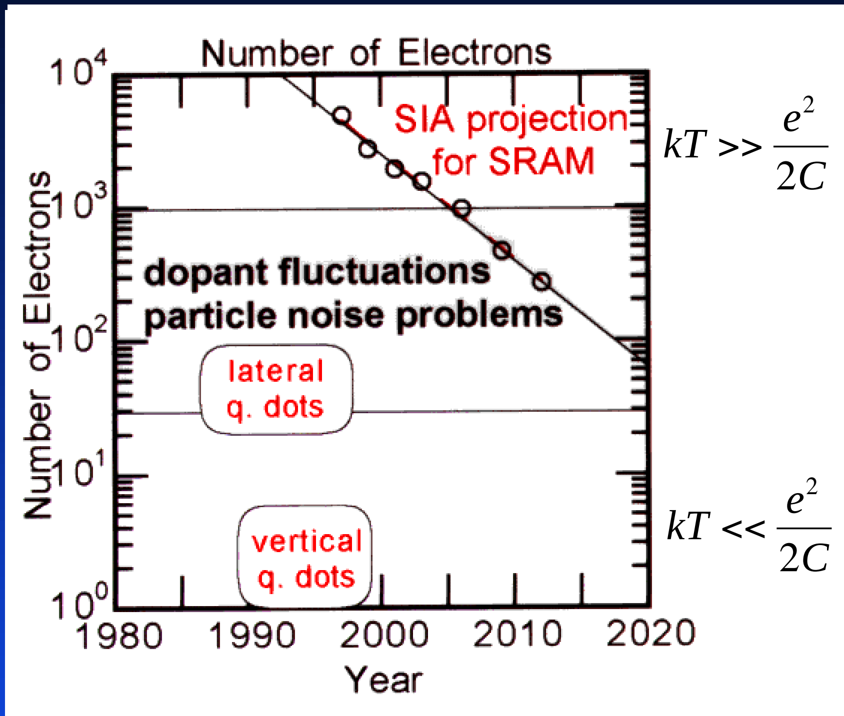


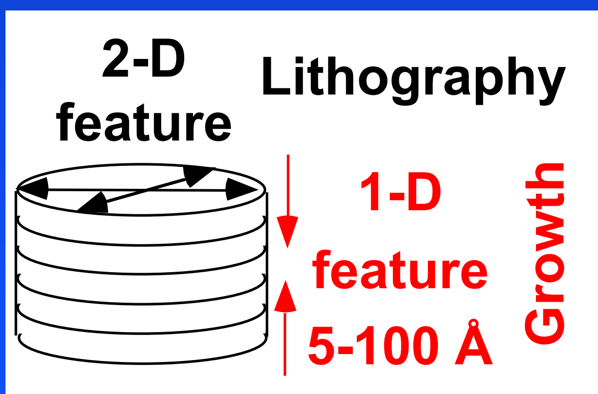
- Moore's Law shows quantum devices in the far future.
- Lithography data alone is deceiving: Layer thicknesses are already on the atomic length scale!
- Commercial devices see quantum limitations:
  - direct tunneling
  - state quantization
- Advanced devices utilize the quantum mechanical behavior:
  - Resonators (RTDs)
  - Active and passive sensors tunable by design - not by material system choice (QWIP).

-> 1D quantum device modeling

-> NEMO

Microdevices Head for Single-Electronics





Reduction of Device Size

↓

Reduction of electron #
Reduction of Capacitance

↓

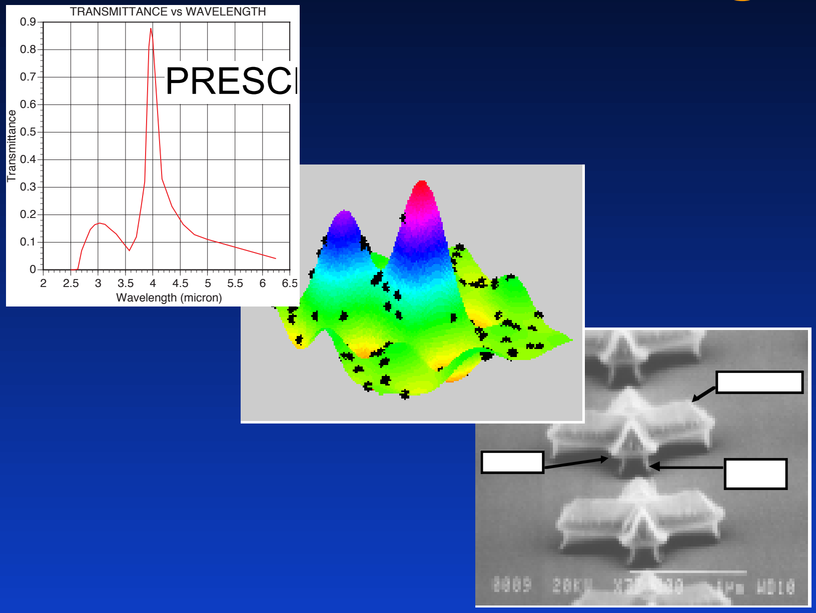
Problem:
Increase in thermal particle noise for tens and hundreds of particles

Solution:
Quantum Dots
Artificial Atoms/Molecules
Single Electronics

↓

System is stable against thermal particle noise

Global Optimization for Microelectronic Device Design



Objective:

- **Synthesis and optimization of microelectronic devices**
- **Limit and focus number of experiments needed to produce design**

Approach:

- Analysis with existing electromagnetic and electronic structure modeling codes
- Apply parallel genetic algorithm library for global optimization
- Use massively parallel platforms to complete designs

Impact:

- Enable device optimization for microelectronic-based missions.
- Near Term:
  - Optimize devices.
- Long Term:
  - Provide instrument-system level optimization

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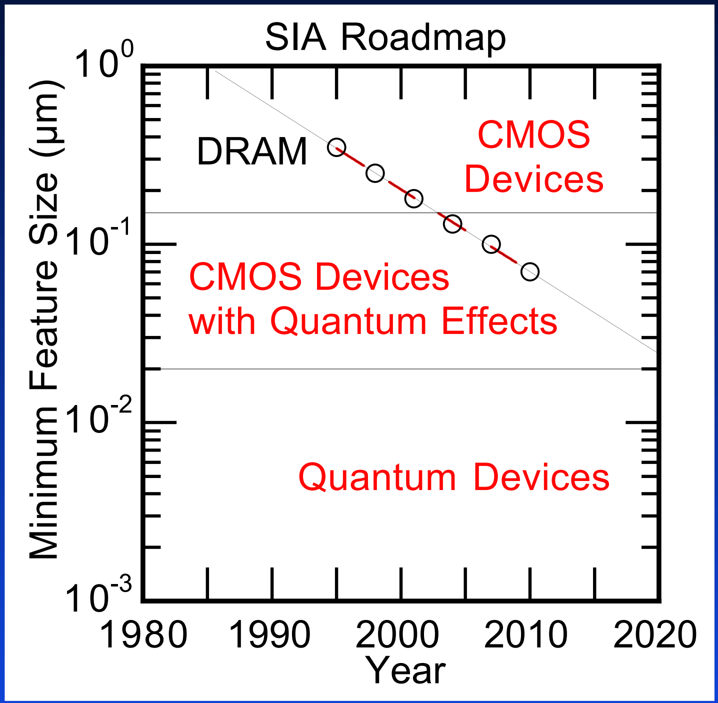
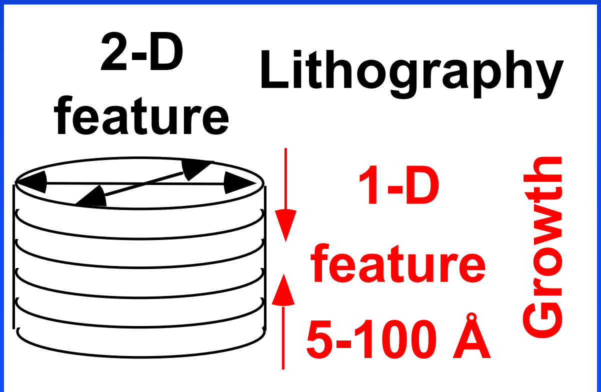
Microdevices Head for Atomic Dimensions





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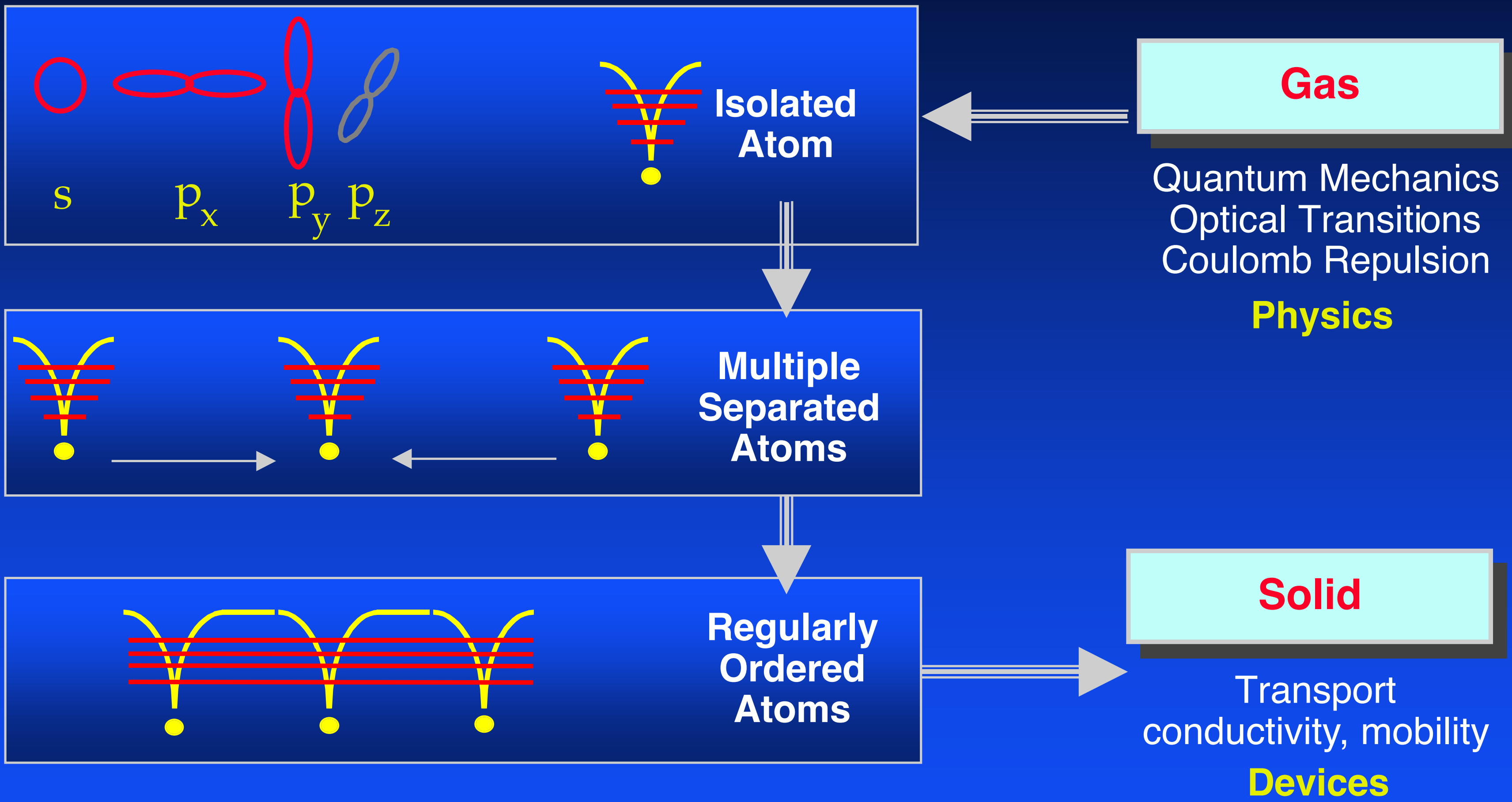
-> 1D quantum device modeling

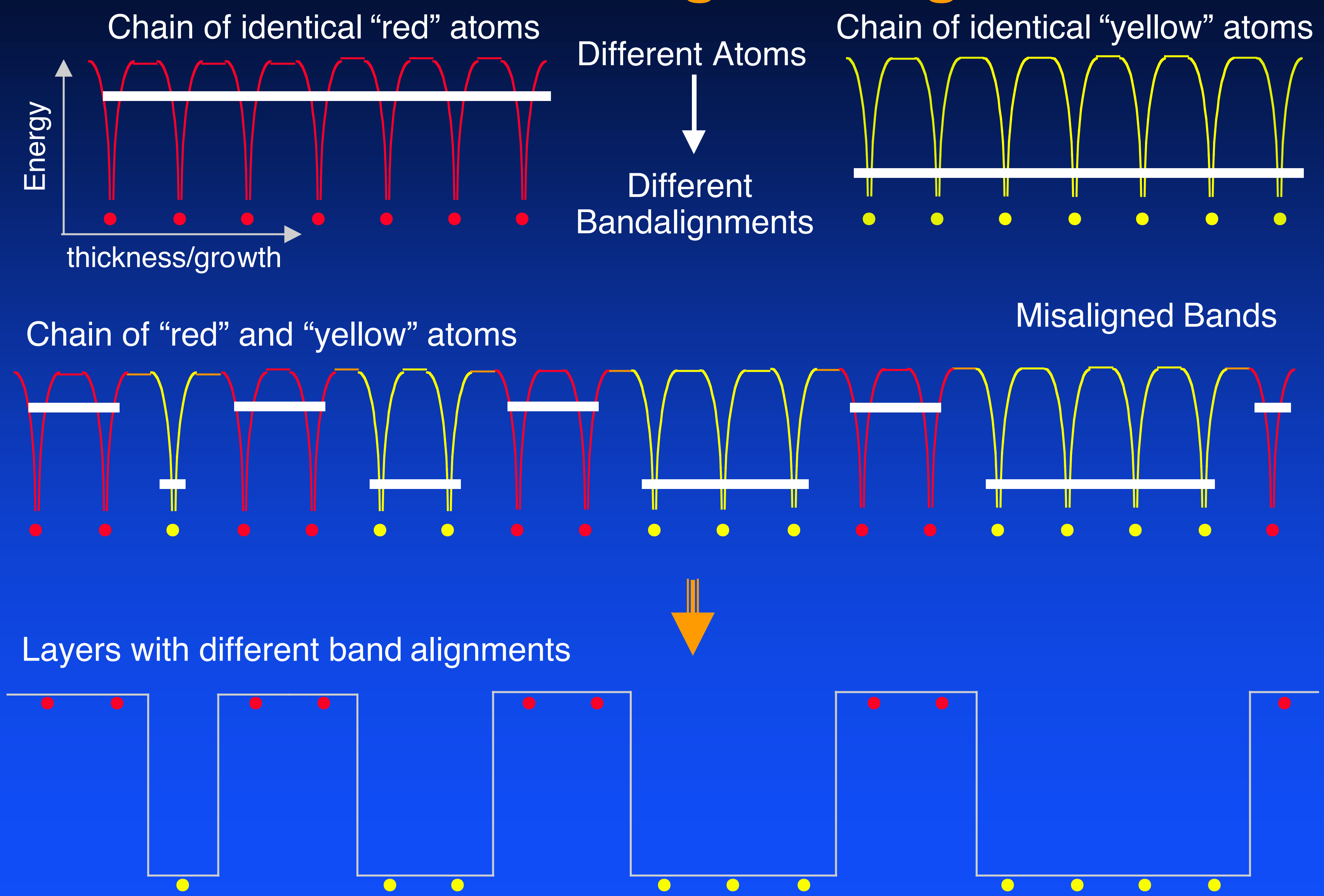
-> NEMO

Bandstructure Basics
Electron Conduction in Solids

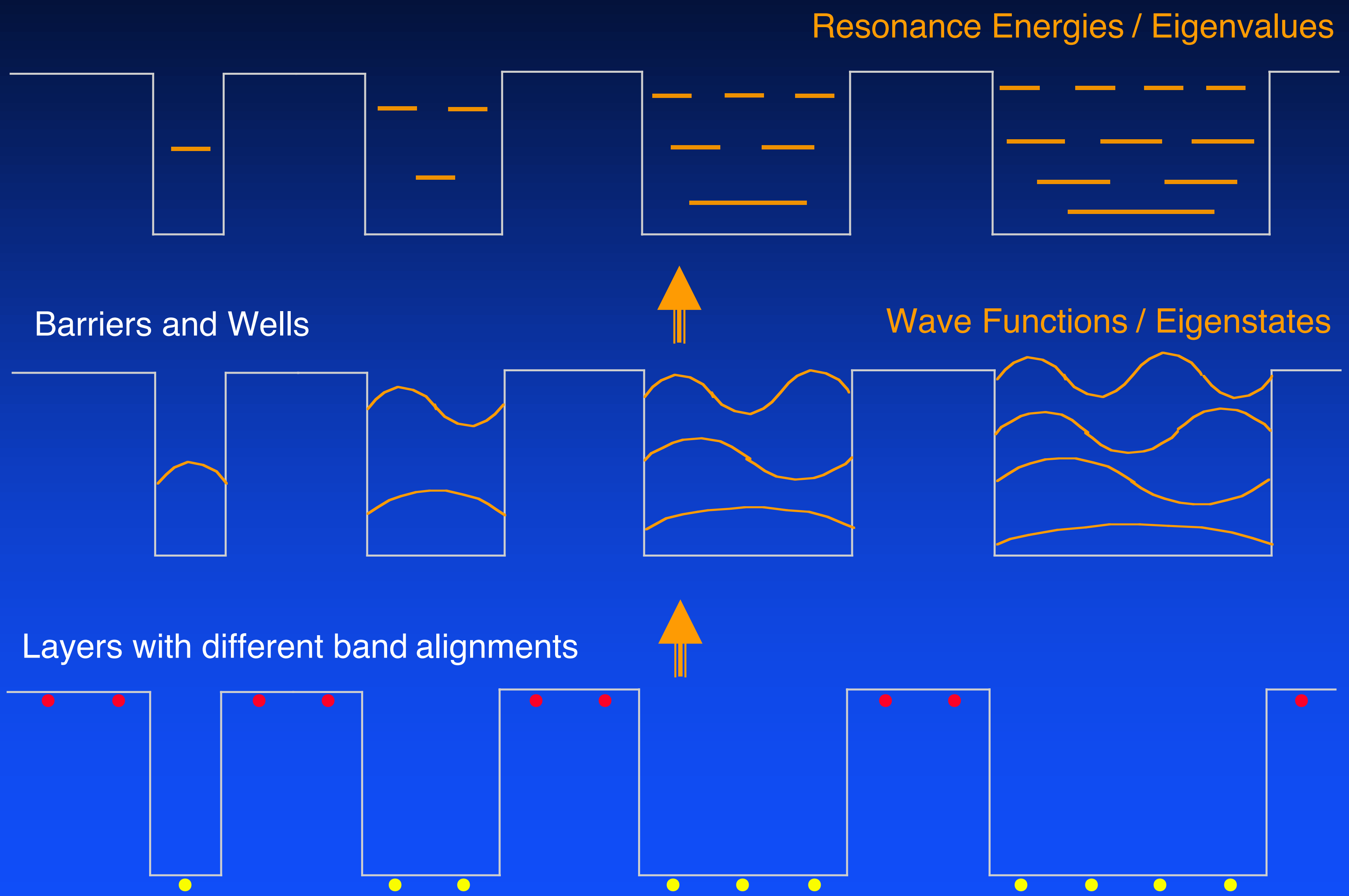


- Bands are channels in which electrons move “freely”.
- Layers of **different** atoms are deposited with **monolayer** control.
- We can **engineer** the electron **bands**.

Bandstructure Engineering Basics



Bandstructure Engineering Basics

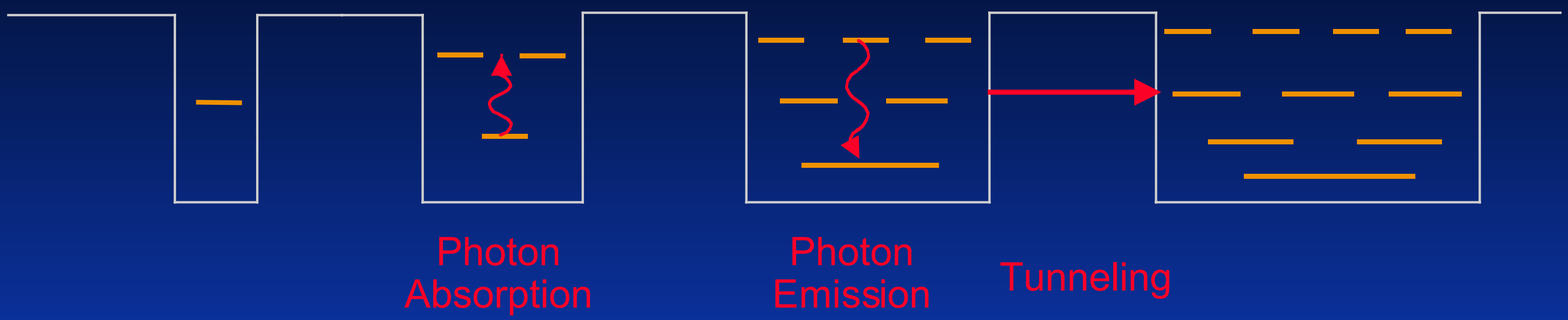


Bandstructure Engineering Basics

Resonance Energies / Eigenvalues

Bandstructure Engineering Applications

Transitions / Transport

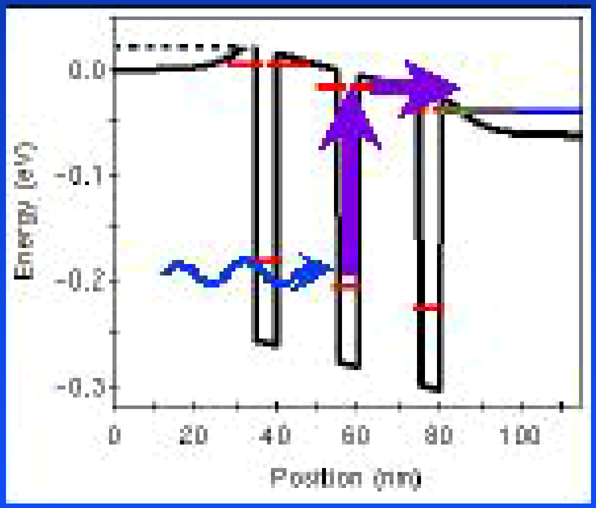


Bandstructure Engineering Applications

Transitions / Transport

Photon
Absorption

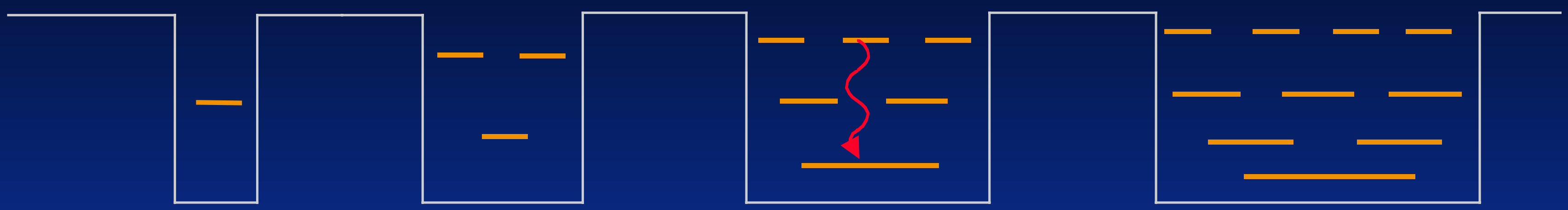
Detectors



Quantum Well
Infrared Detector

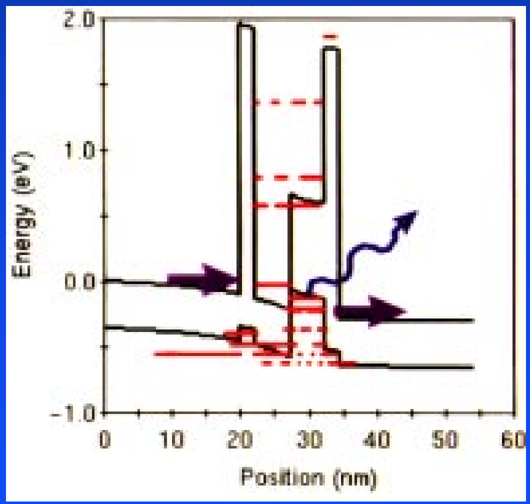
Bandstructure Engineering Applications

Transitions / Transport



Photon Emission

Lasers



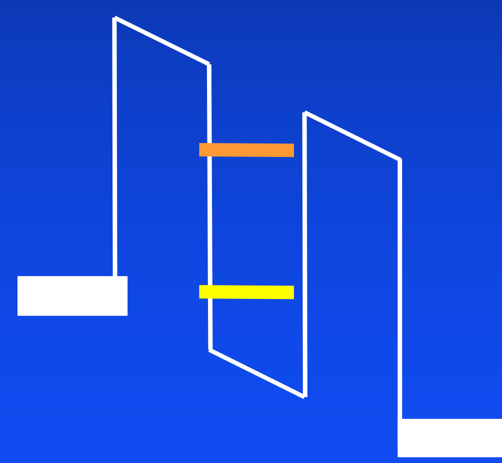
Quantum Cascade Laser

Bandstructure Engineering Applications

Transitions / Transport

Tunneling

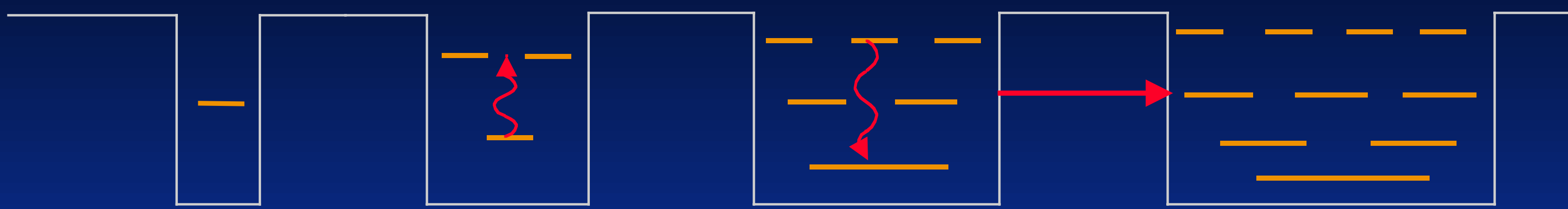
Logic / Memory



Resonant
Tunneling
Diode

JPL

Transitions / Transport Controlled by Design



Photon Absorption

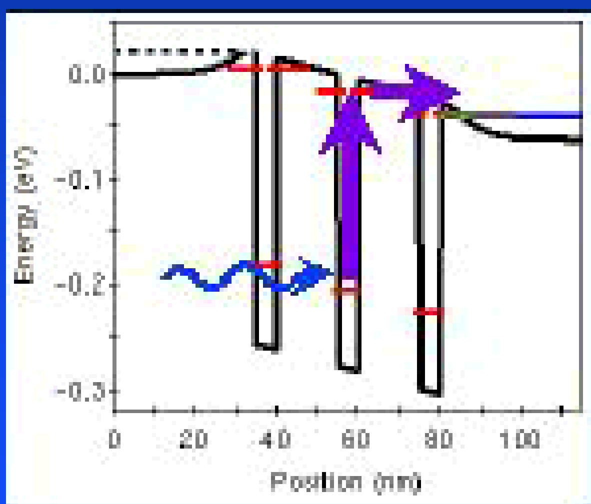
Photon Emission

Tunneling

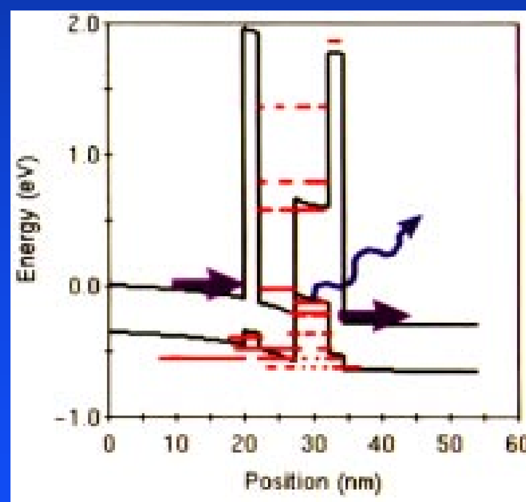
Detectors

Lasers

Logic / Memory



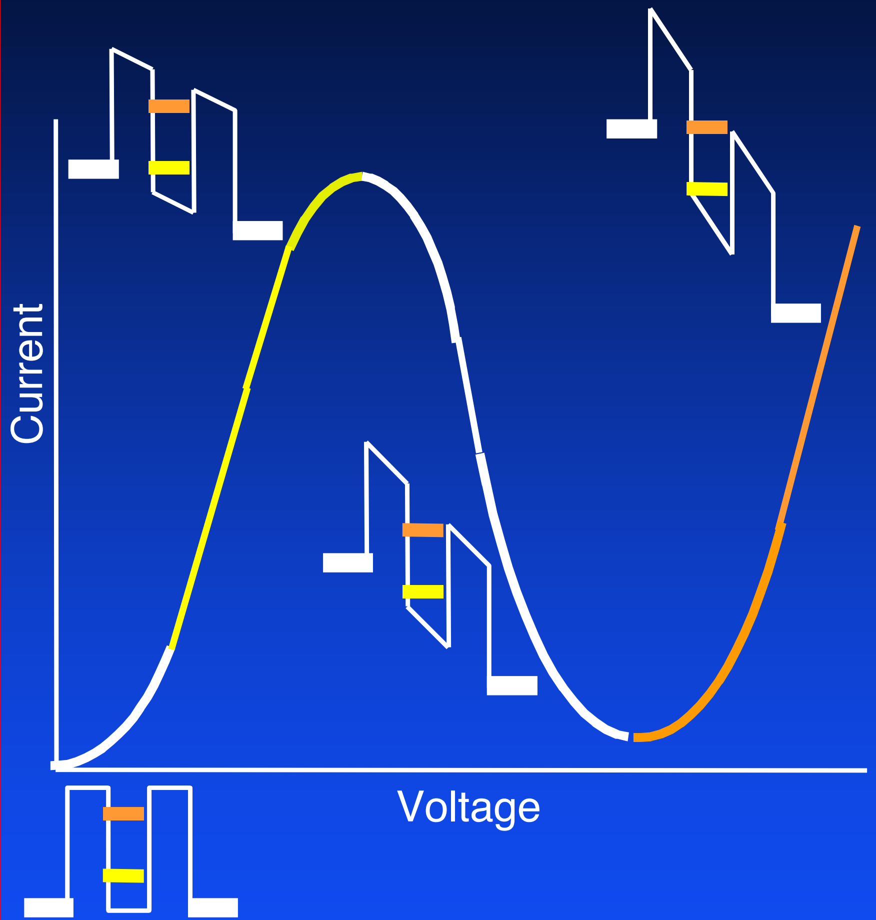
Quantum Well Infrared Detector



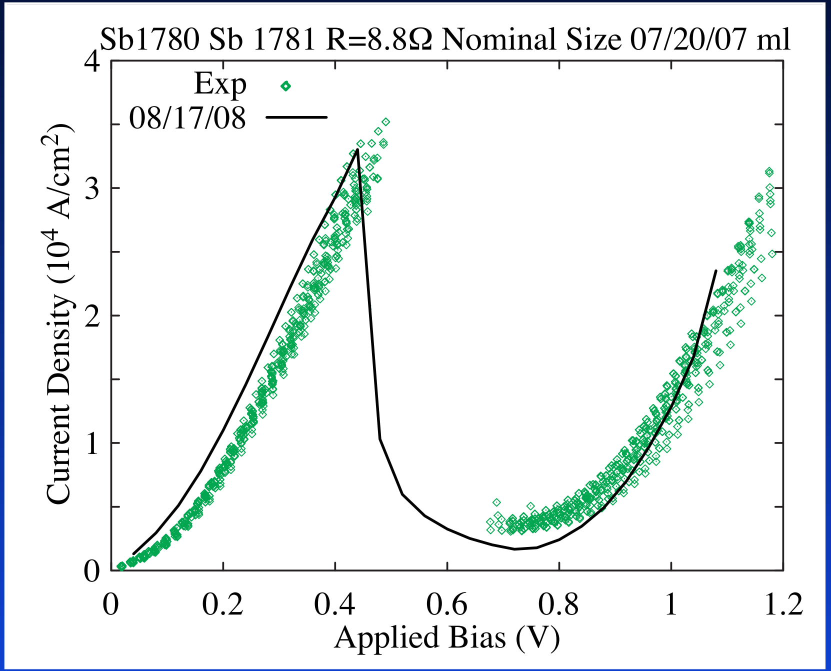
Quantum Cascade Laser

Resonant Tunneling Diode

Resonant Tunneling Diode



Conduction band diagrams
for different voltages
and the resulting current flow.



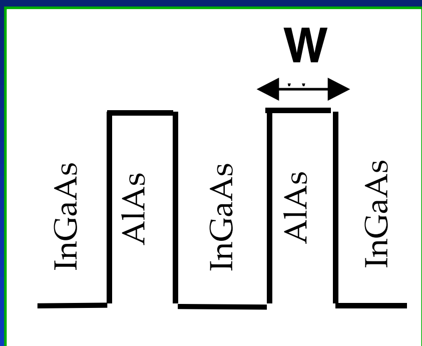
12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

50nm	1e18	InGaAs
7 ml	nid	InGaAs
7 ml	nid	AlAs
20 ml	nid	InGaAs
7 ml	nid	AlAs
7 ml	nid	InGaAs
50 nm	1e18	InGaAs

NanoElectronic MOdeling (NEMO) Simulation

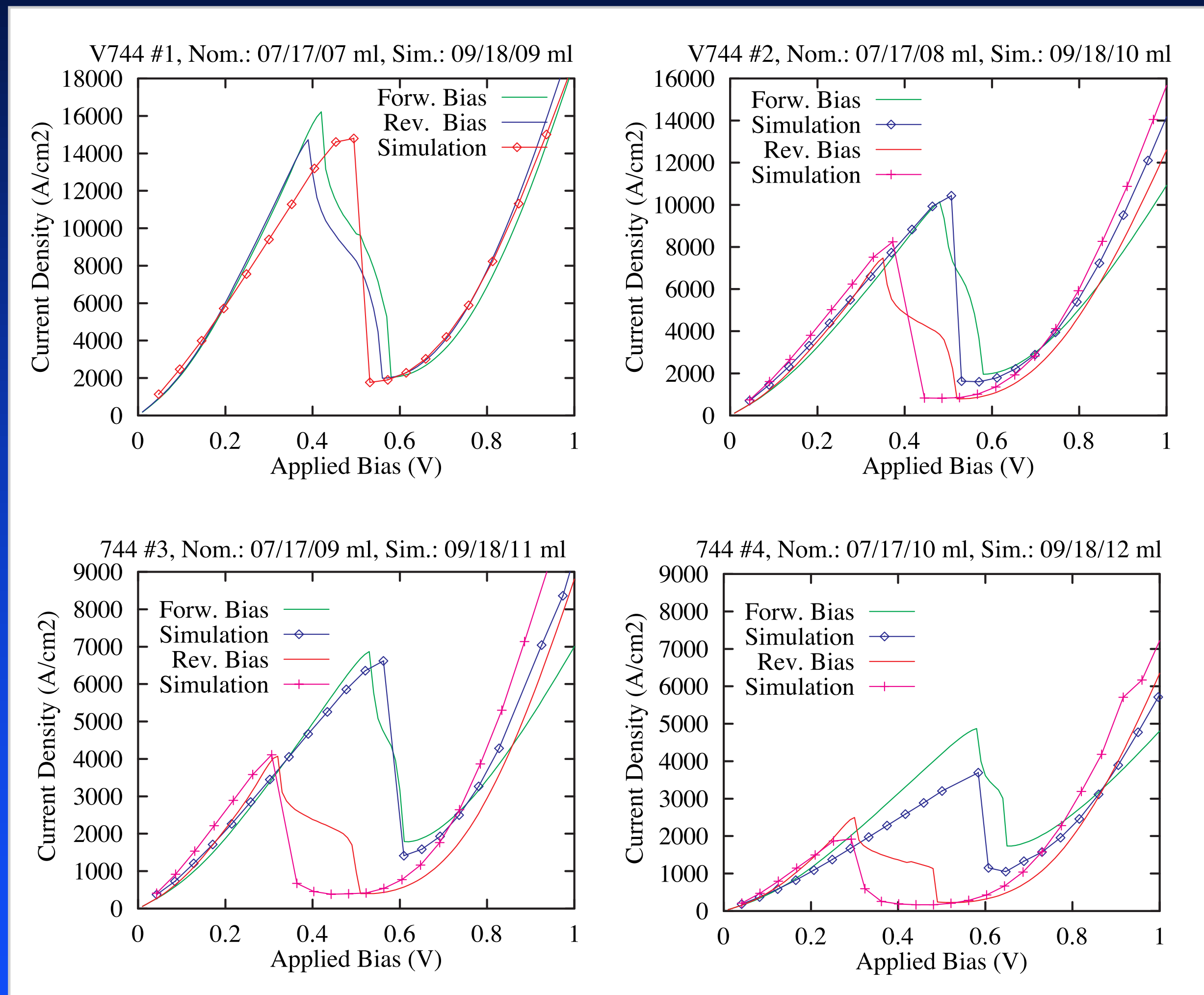
Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

Vary One Barrier Thickness



Four increasingly asymmetric devices:

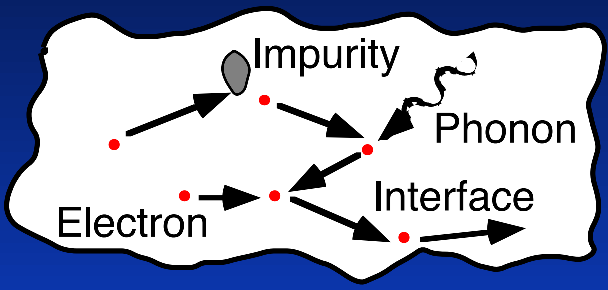
20/50/20 Angstrom
20/50/23 Angstrom
20/50/25 Angstrom
20/50/27 Angstrom



Presented at IEEE DRC 1997, work performed at Texas Instrument, Dallas

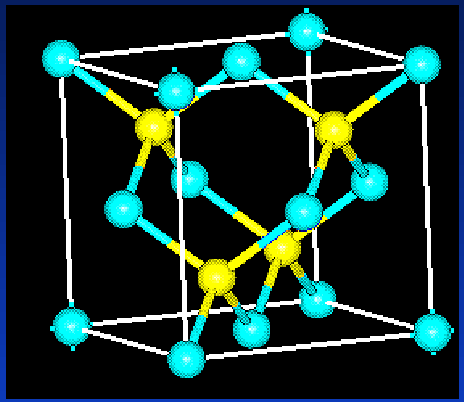
Where is NEMO compared to other models?

What is Needed for Quantum Electron Transport?



NEMO

Charging
Bandstructure
Scattering
Interference



Drift-Diffusion
Boltzmann Eq.

Non-Equilibrium
Green Functions

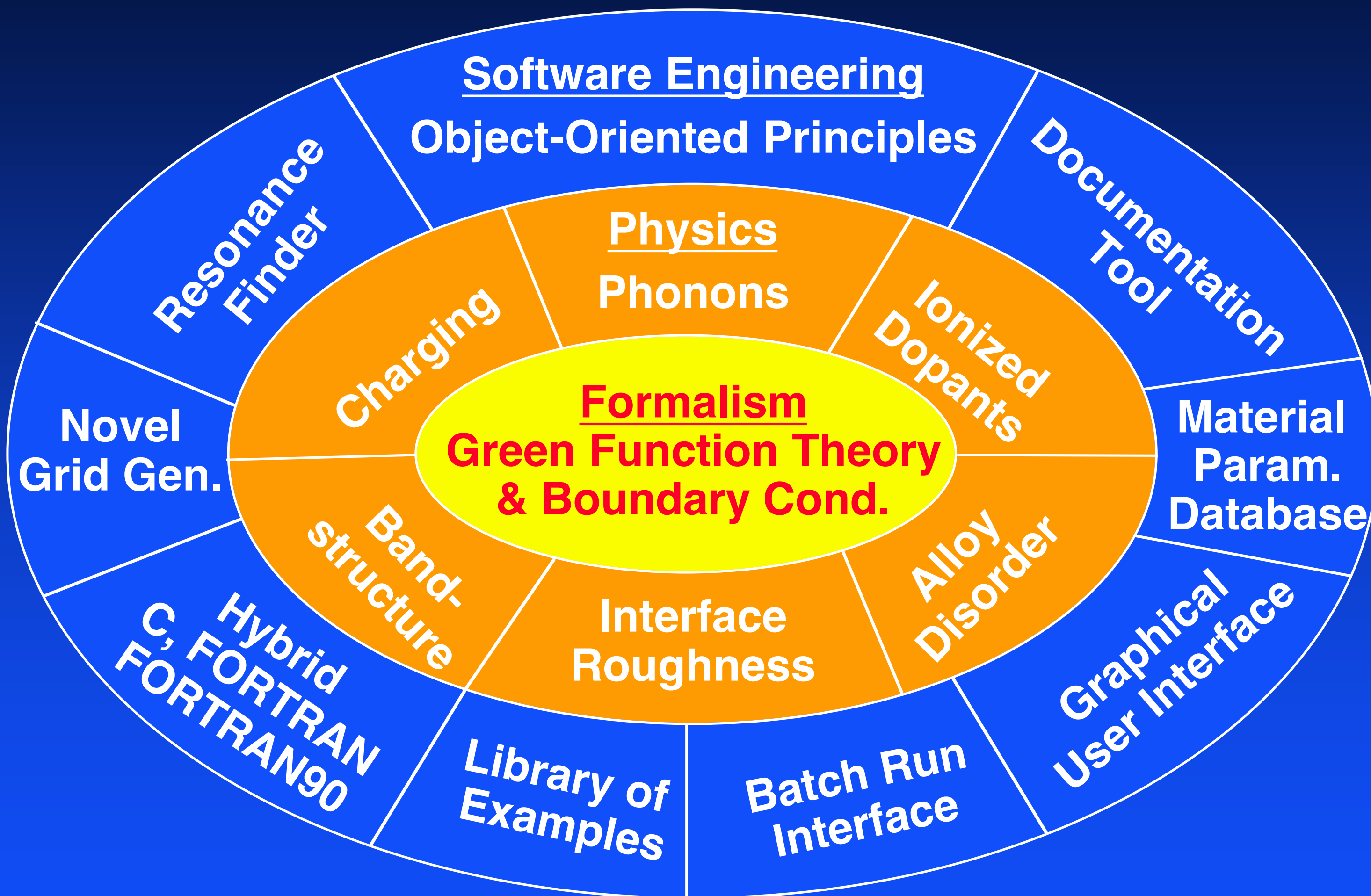
Schrödinger
Equation

Transport with particle interaction

Quantum Mechanics

NEMO: A User-friendly Quantum Device Design Tool

Formalism, Physics, and Technology



Approximately 250,000 lines of code

NEMO Genealogy

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-1997
  - Theory
    - Roger Lake, Chris Bowen, Gerhard Klimeck, Tim Boykin (UAH)
  - Graphical User Interface
    - Dan Blanks, Gerhard Klimeck
  - Programming Approach, Philosophy, and Prototypes
    - Bill Frensley (UTD), Gerhard Klimeck, Chris Bowen
  - Coding Help
    - Manhua Leng (UTD), Chenjing Fernando, Paul Sotirelis, Dejan Jovanovic, Mukund Swaminathan (UTA),
  - Experiments for verification
    - Ted Moise, Alan Seabaugh, Tom Broekaert, Berinder Brar, Yung-Chung Kao

- Gerhard Klimeck and Chris Bowen were the core developers. They are both with JPL now.

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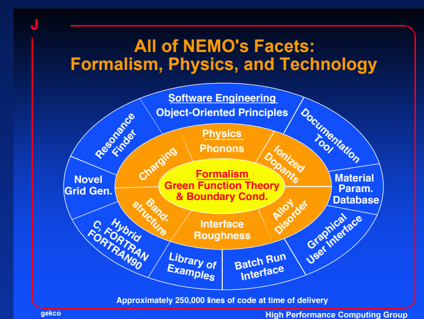
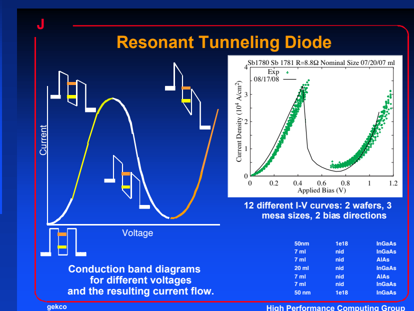
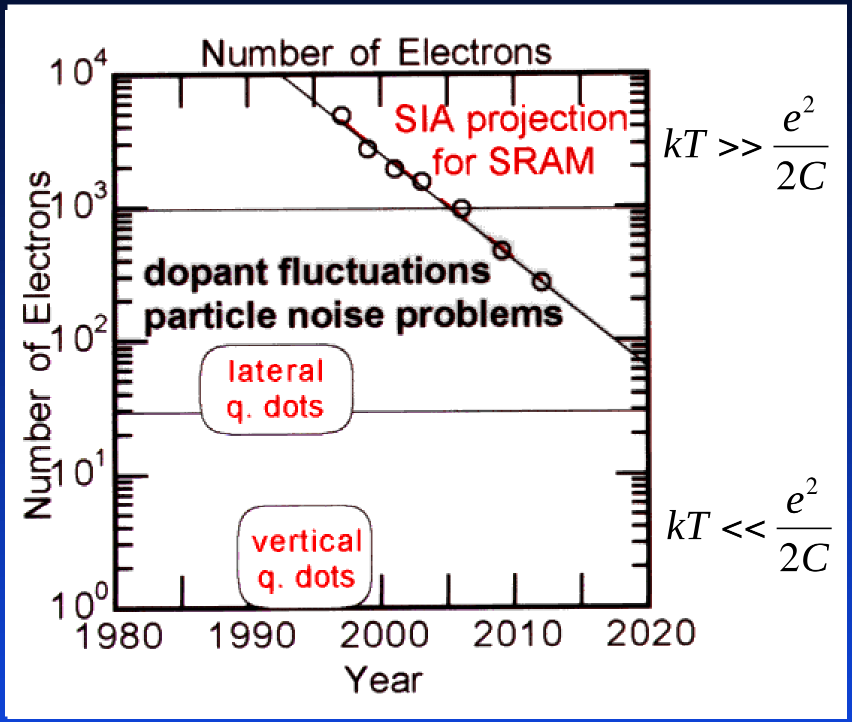
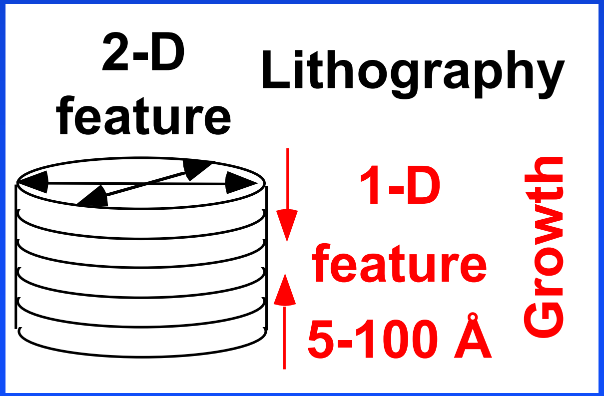




Microdevices Head for Single-Electronics





Reduction of Device Size

↓

Reduction of electron #
Reduction of Capacitance

↓

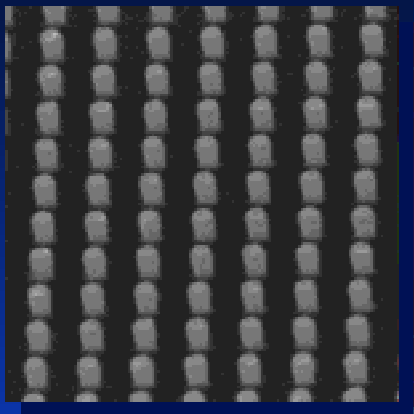
Problem:
Increase in thermal particle noise for tens and hundreds of particles

Solution:
Quantum Dots
Artificial Atoms/Molecules
Single Electronics

↓

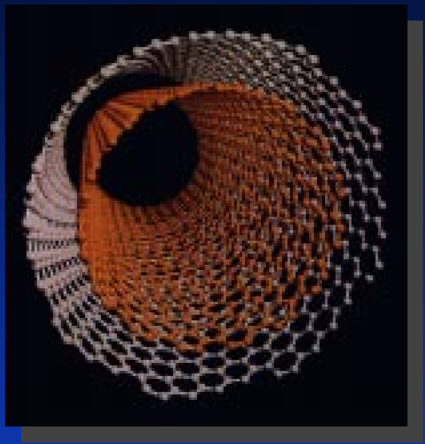
System is stable against thermal particle noise

Examples of 3D Confined Structures



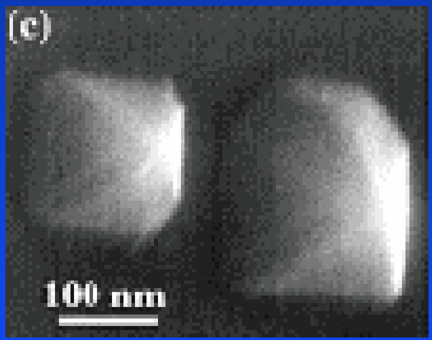
Quantum Dots:
Litho-based, GaAs/AlGaAs, InGaAs/InAlAs systems

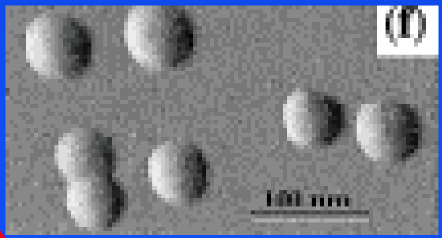
Cylinder shaped
M Reed et al, TI (1988)



Fullerenes, C60:
Carbon based
Electronic and mechanical appl.

Rice Univ.,
NASA Ames

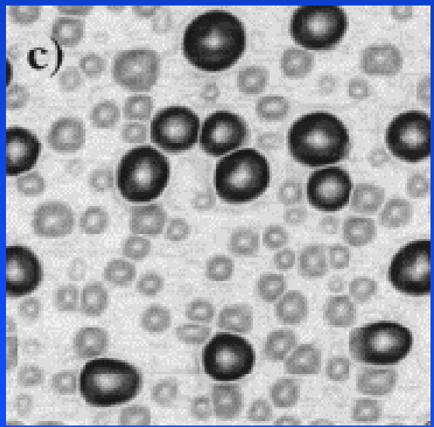




Quantum Dots:
Self-assembled , InAs on GaAs.

Pyramidal or dome shaped

R. Leon et al,
JPL (1998)



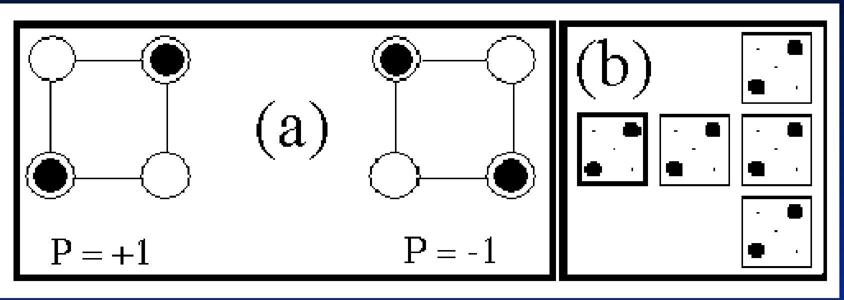
Quantum Dots:
Self-assembled , Ge on Si.

Dome shaped

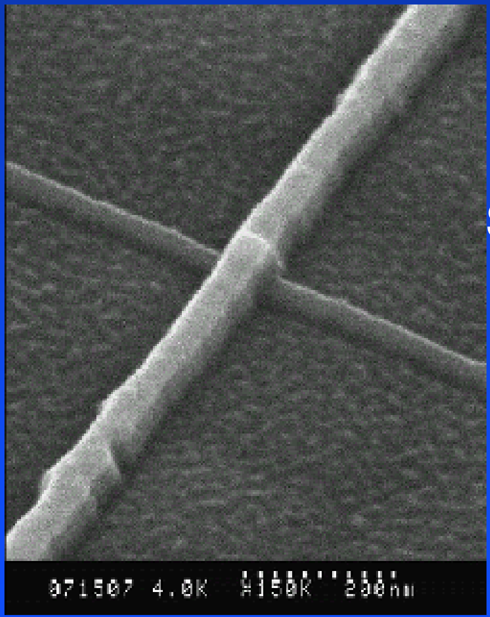
S. Williams et al,
HP (1998)

Quantum Dots Applications

- **Memory:**
  Store discrete charge in potential wells.
- **Transistors:**
  Use discreteness of channel conduction.
- **Logic:**
  Use electrostatically coupled quantum dots.

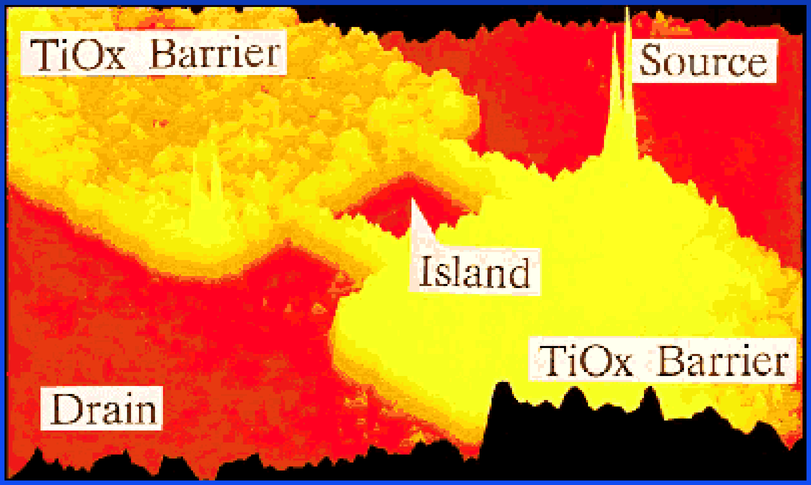


Lent, Porod @ Notre Dame: Quantum Cellular automata, electrostatically coupled quantum dots.



Chou @ Princeton Room Temp. Single Electron Memory

Hitachi: 128Mbit Integration demonstrated

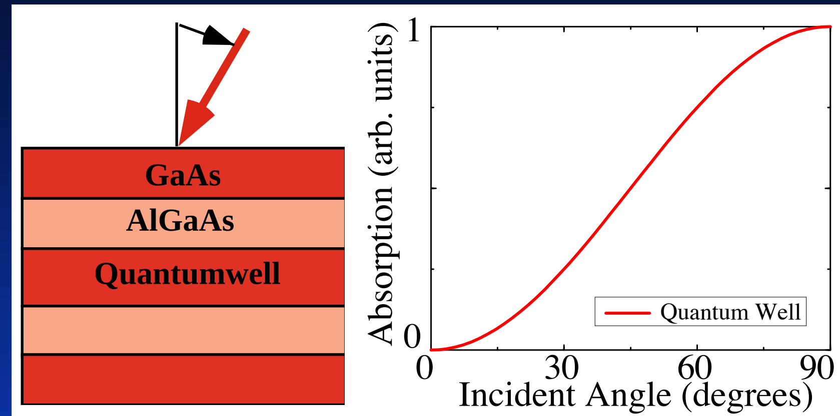


Harris @ Stanford: Room temperature single electron transistor

Quantum Dots as Optical Detectors

Desensitizing QWIP to Polarization

- **Problem:**
  Quantum wells are "blind" to light impinging orthogonal to the detector surface.
- **Standard Solution:**
  Use gratings to turn polarization
- **New Approach:**
  Quantum dots have a built-in anisotropy and state quantization in all three dimensions
  -> absorption at all angles

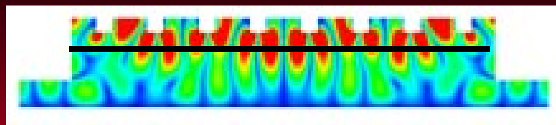


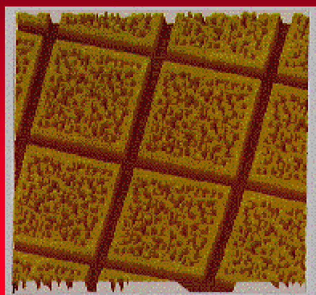
Quantum Wells: Absorption has strong incidence angle dependence

Standard Solution:

Grating

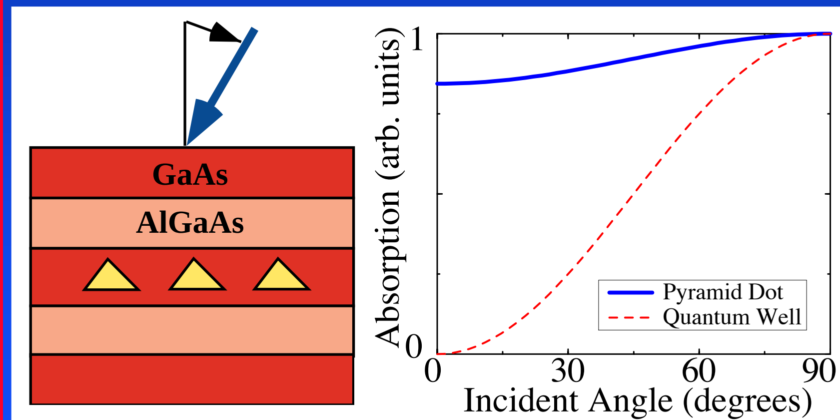
Electromagnetic Modeling





electric field models

optimized light coupling



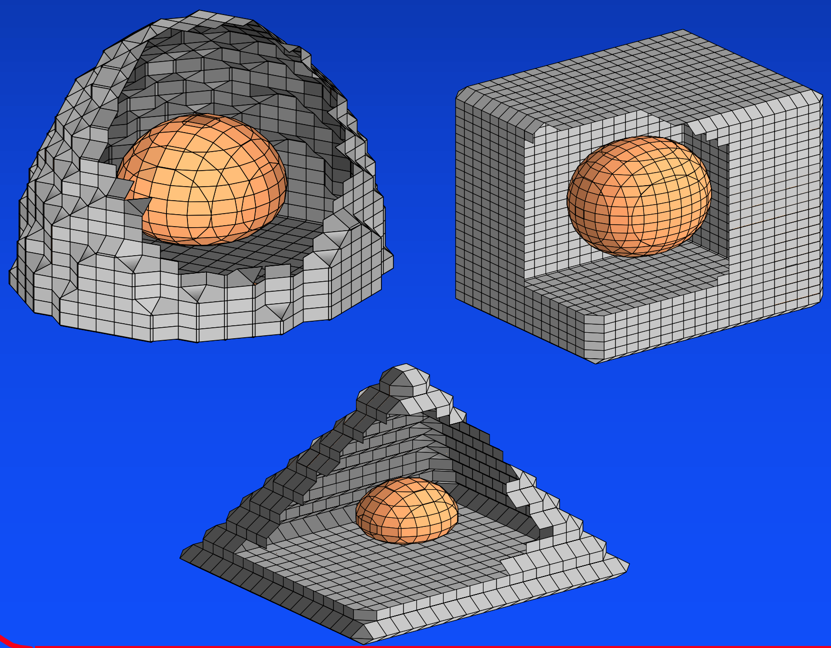
Quantum Dots: Absorption has weak incidence angle dependence

Development of a 3D Quantum Simulator

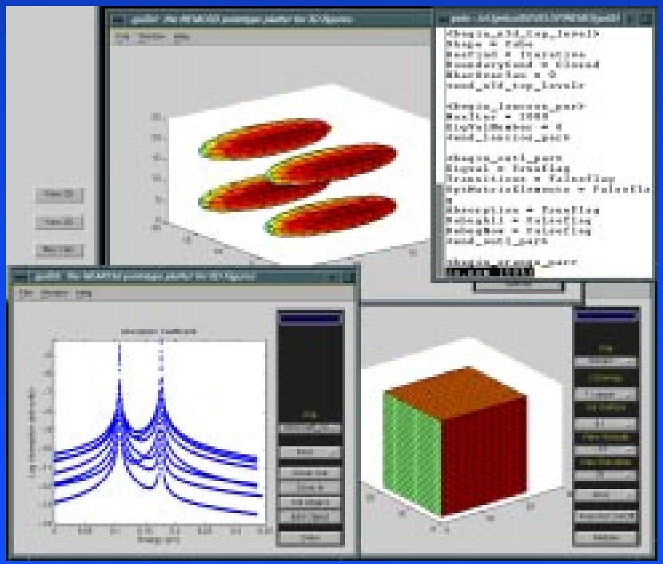
Problem:
- Develop quantum dot based technologies for digital and optoelectronic applications.

Approach:
- Deliver a graphically driven quantum dot design tool.
- Leverage JPL's strength in massively parallel computation.

Impact:
- Near Term - Optical Detection:
  - Guidance for choice of sizes, materials, shapes.
  - Optimize optical absorption.
- Long Term:
  - Provide general modeling tools for the analysis of ultra-scaled structures.



We are toolmakers!



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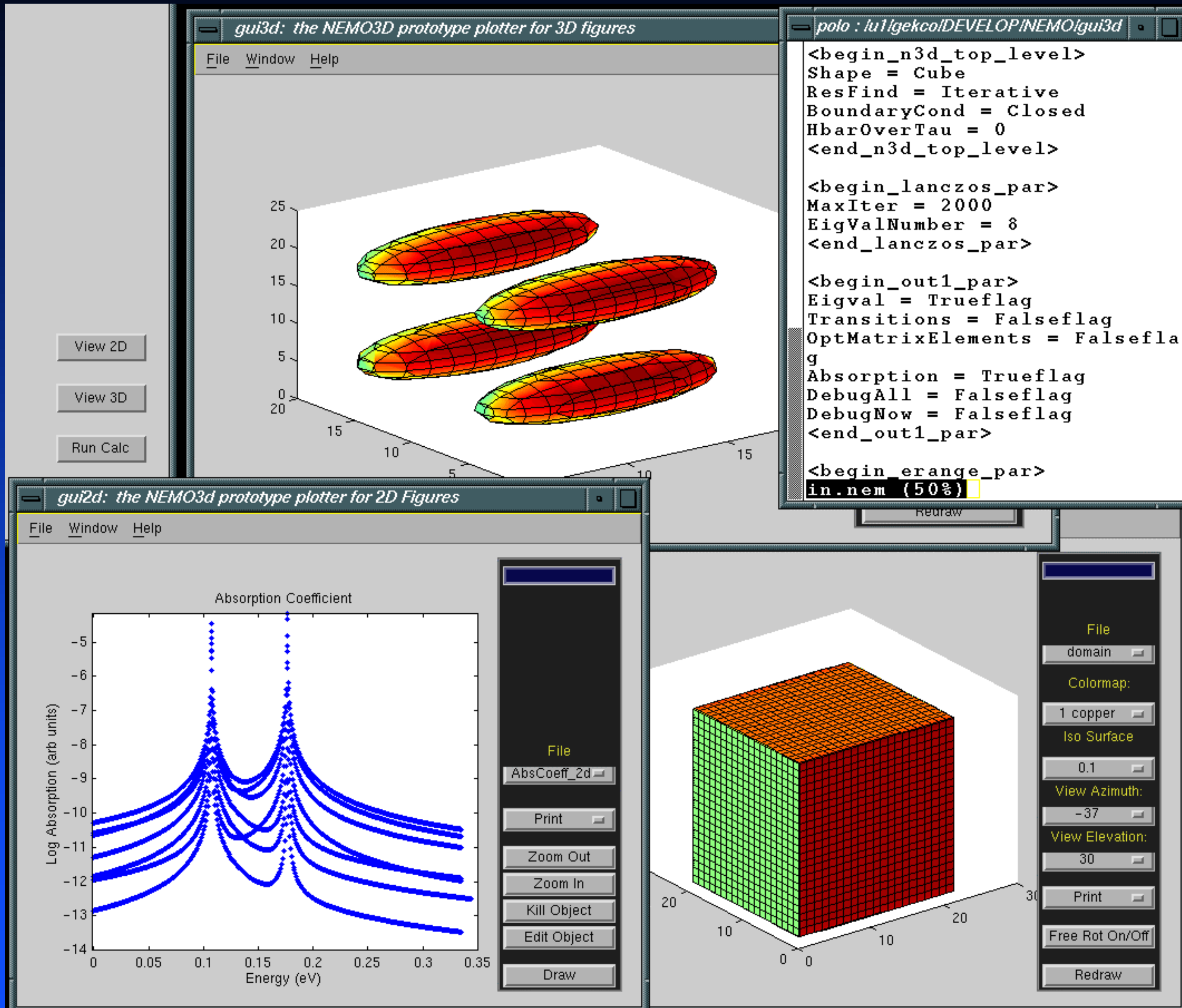
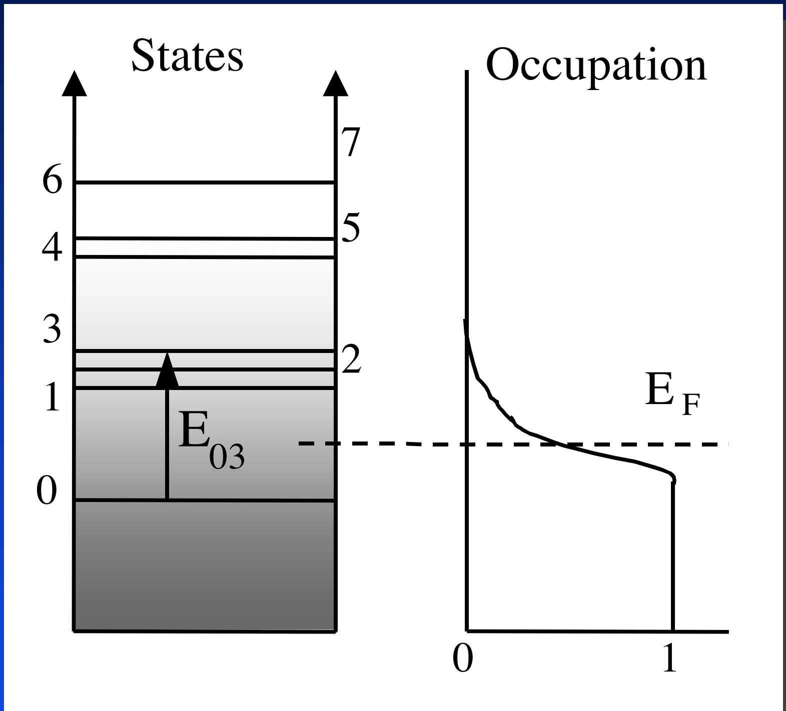
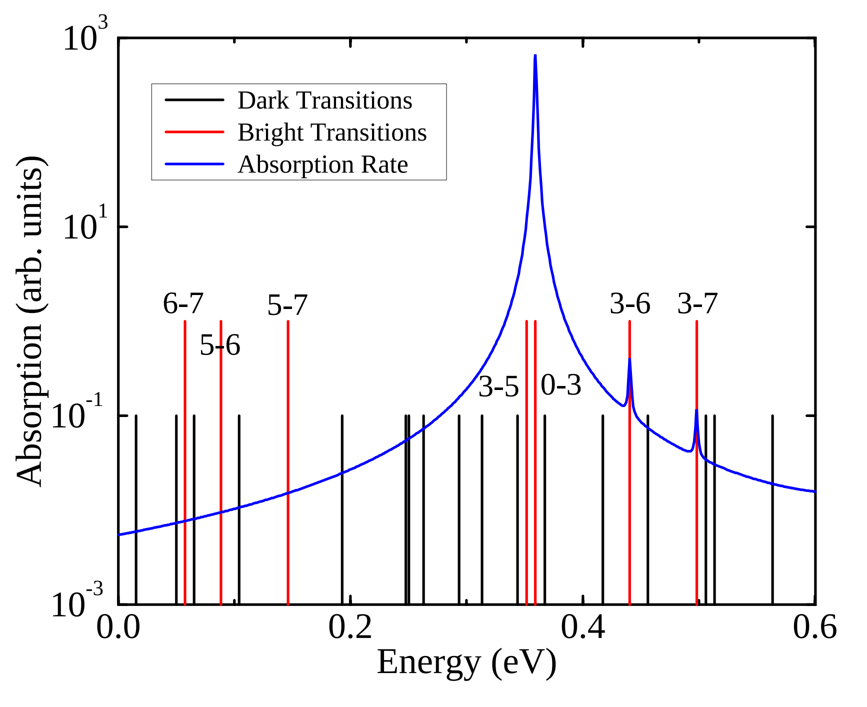


Optical Absorption in a Pyramidal Dot

State Occupation



Absorption vs Energy

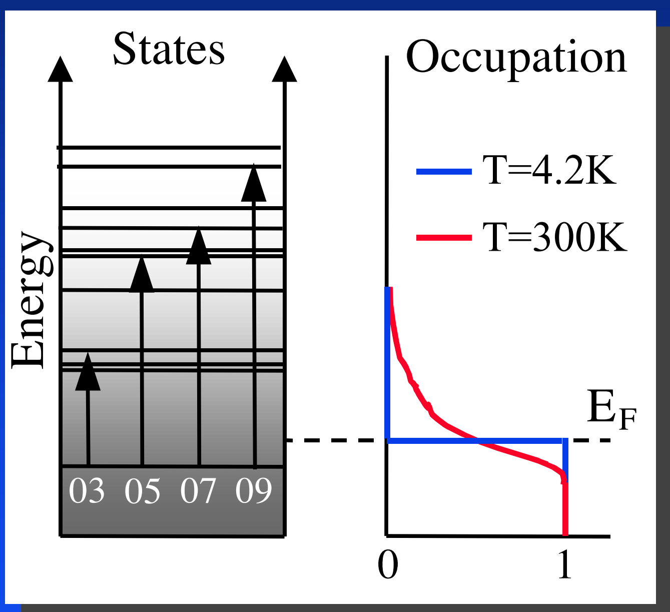


Two Issues influence the absorption strongly:

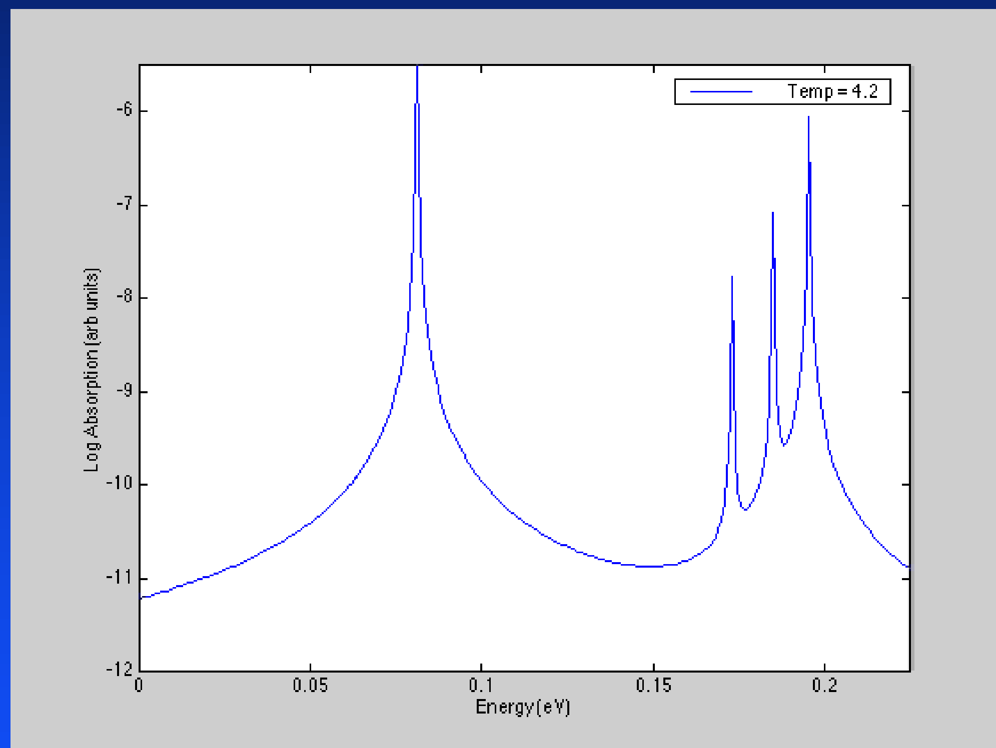
- **Only the lowest 4 states contain electrons, so transitions between higher states do not result in optical absorption.**
- **Bright transitions occur between states that posses opposite parity in the direction of the optical field.**

Temperature Dependence of Quantum Dot Absorption Spectrum

State Occupation



Absorption



Higher temperatures => More occupied states => More transitions.

Summary - After 2 Months of Work

Achievements:

- Prototyped general eigenvalue solver which scales as order $N^{1.1}$ rather than N^3.
- Solved $N=10^6$ grid point problem on 1 CPU in 1 hour.
- Developed graphical interface prototype.

Future Resource Requirements:

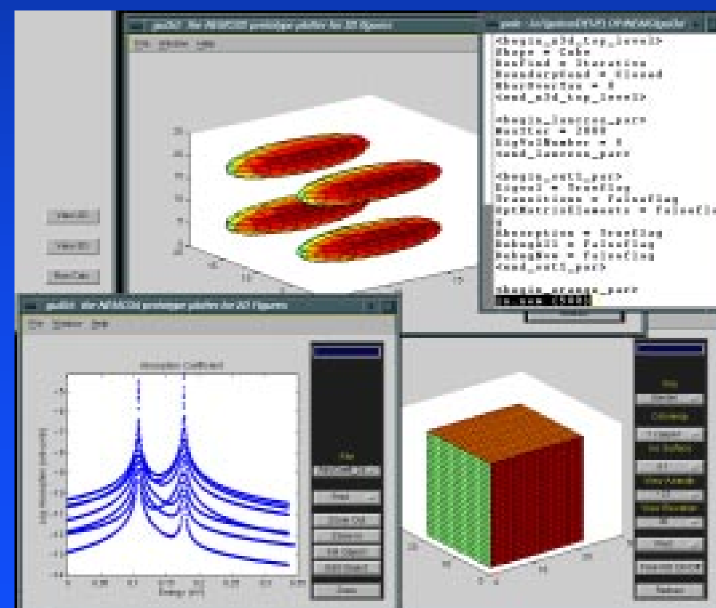
- Bandstructure models cause 400x increase in required CPU time.
  -> computation is CPU not memory limited
  -> need massively parallel machines with good wall-clock turn-around
- Engineering optimization/evolution will require thousands of runs
  -> need next generation supercomputer

Plans:

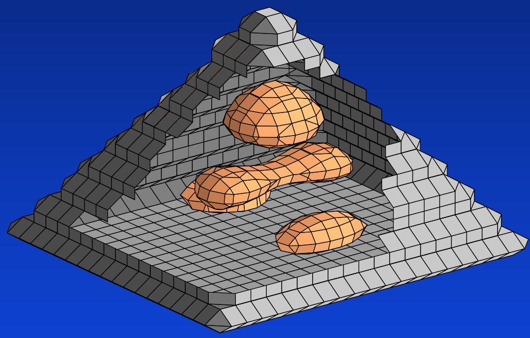
- Incorporate mechanical strain.
- Incorporate sp3s* and sp3d5 bandstructure models.
- Electron charging effects.

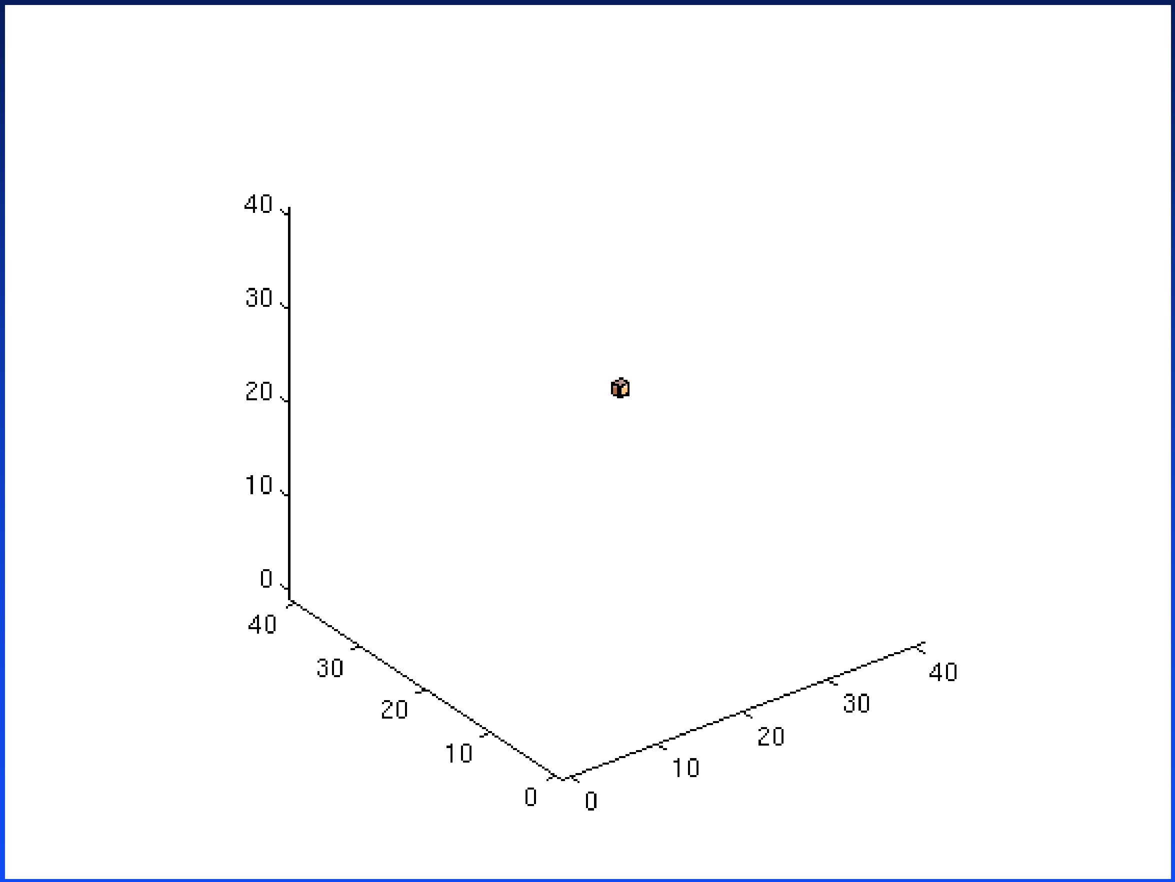
- Prototype parallel version of eigenvalue solver.
- Prototype client-server approach to interface graphical user interface to supercomputers.

We are toolbuilders



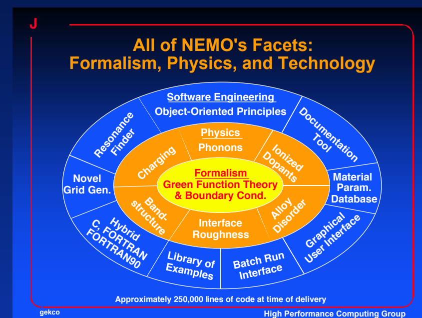
Animation of the 7th Eigenstate in a Pyramidal Quantum Dot

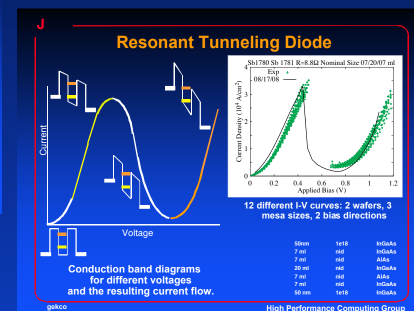


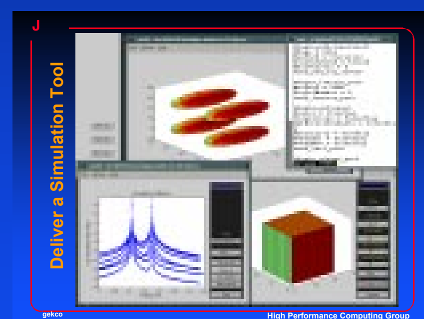


Simulator Development for Nanoelectronic and Electromagnetic Devices

- **Motivation**
- **1D modeling**
  - Bandstructure
  - Resonant Tunneling
  - NEMO
- **3D modeling**
  - Quantum Dots
  - NEMO-3D
- **Design and Synthesis**
  - **GENES (Genetically Engineered Nanostructured Devices)**
- **Future Efforts**
- **Conclusions**







Global Optimization for Microelectronic Device Design

Genetically Engineered NanoElectronic Structures: GENES

Objective:

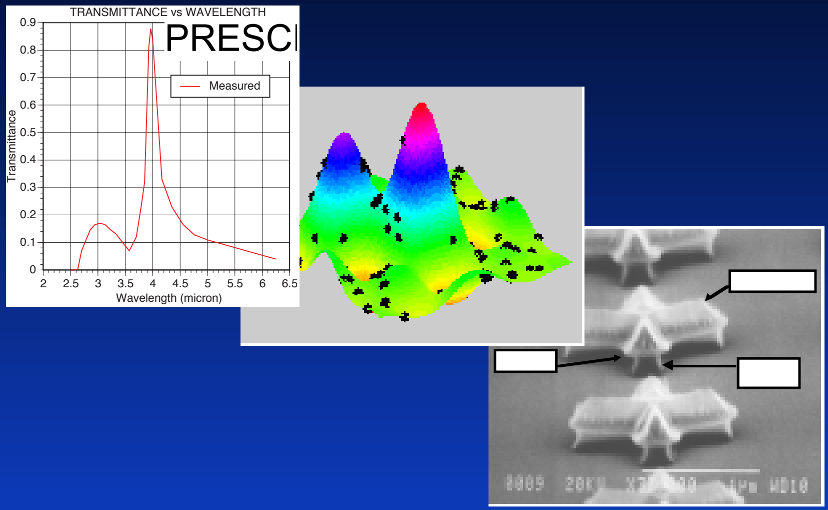
- Optimize and synthesize electronic devices
- Limit and focus number of experiments needed to produce design.

Approach:

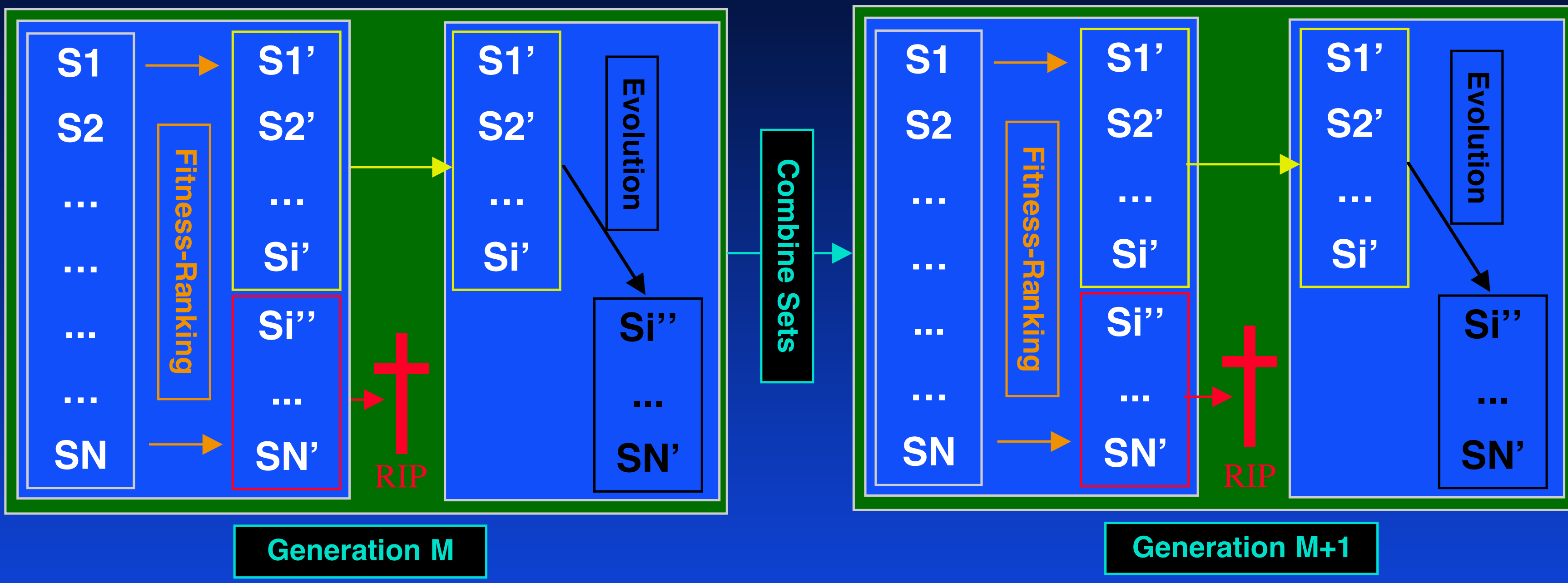
- Use existing electromagnetic and electronic structure modeling codes
- Apply genetic algorithm for global optimization
- Use massively parallel platforms

Impact:

- Enable device optimization for microelectronic-based missions.
- Near Term:
  - Optimize devices.
- Long Term:
  - Provide instrument-system level optimization



Basic Genetic Algorithm



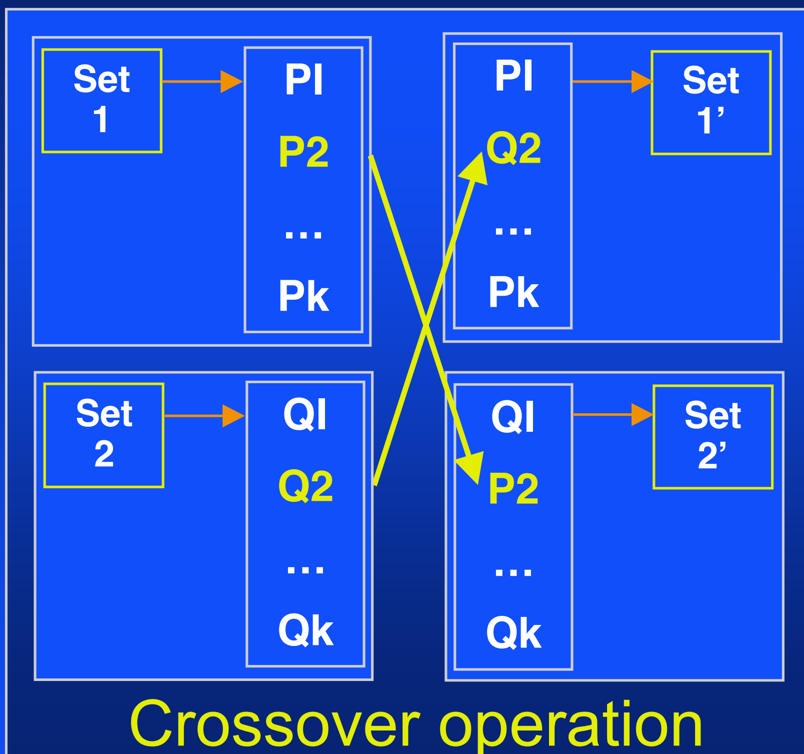
- Genetic algorithm parameter optimization is based on:
  - Survival of good parameter sets
  - Evolution of new parameter sets
  - Survival of a diverse population

- Optimization can be performed globally, rather than locally.

Basic Evolution Operations

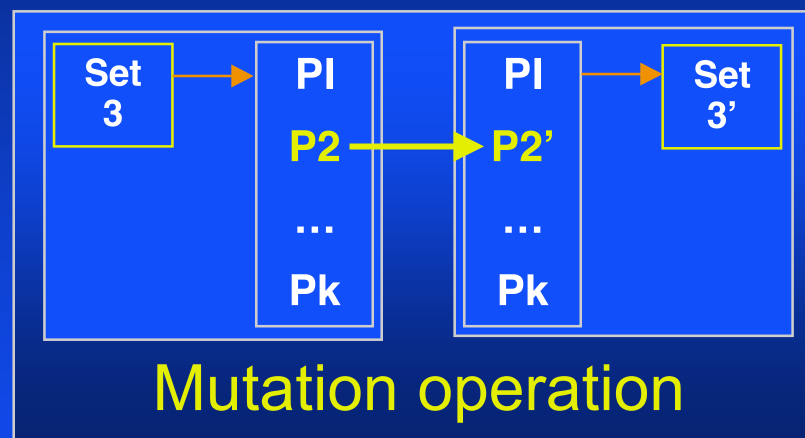
- Each set (Si) consists of several parameters (Pj)
- The parameters Pj can be of different kinds: real, integers, symbols, ….

Gross Exploration



- Crossover explores different combinations of existing genes.

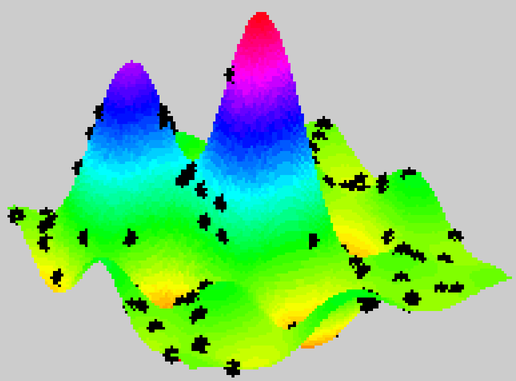
Fine Tuning

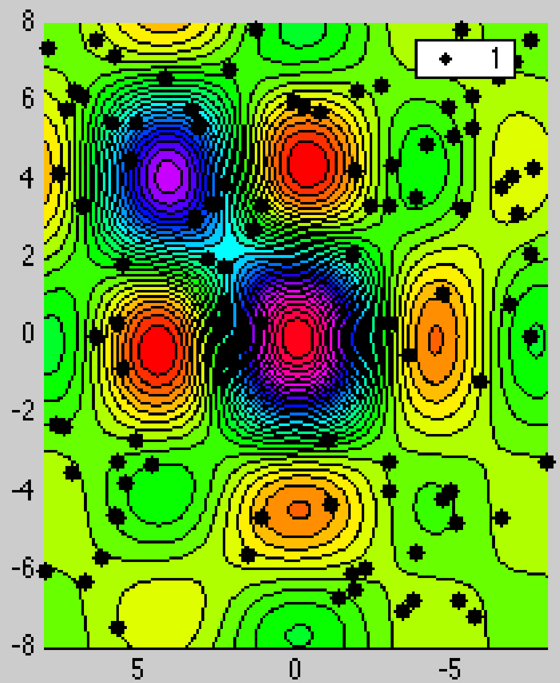


- Creation of new gene values.

Global Optimization via Genetic Algorithms

$$F(x,y) = \frac{\sin(x)}{x}\frac{\sin(y)}{y} + 0.7\,\frac{\sin(x-4)}{(x-4)}\frac{\sin(y-4)}{(y-4)}$$



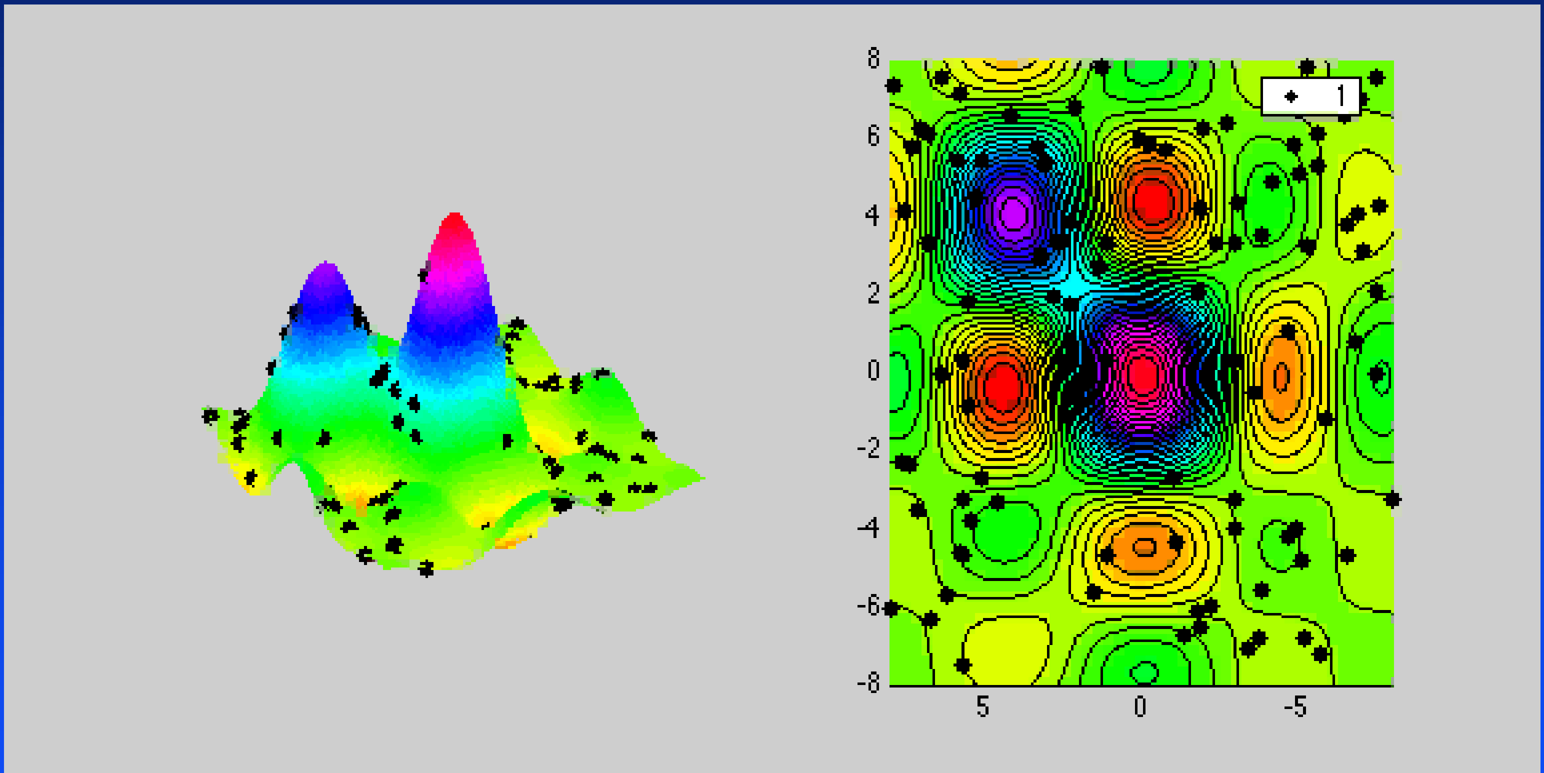


gekco

Global Optimization: Genetic Algorithm Development

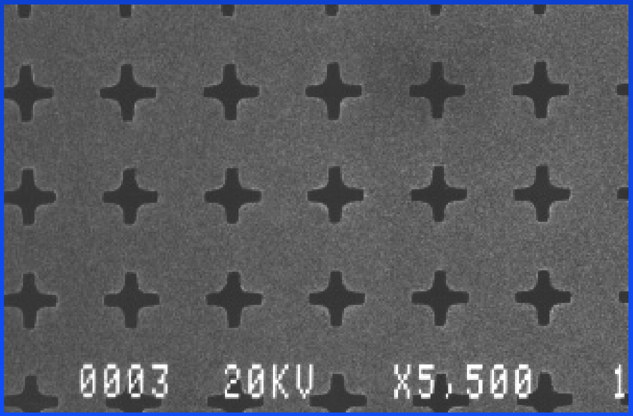
Genetic Algorithm Convergence

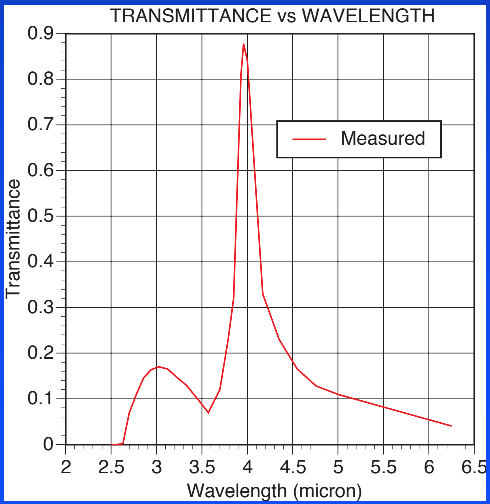
pop = 100, 300 generations, steady-state (10%), 2-point crossover p = 0.85, mutatation p = 1/2



Optical Filters with Patterned Arrays
(Frequency Selective Surfaces-FSSs)

- **E-beam lithography enables:**
  - **Sub-micron resolution in fabrication, allowing infrared filtering**
- **Design requires:**
  - **Tailoring of passbands for specific application**
  - **Understanding of element size and shape, periodicity, and materials.**

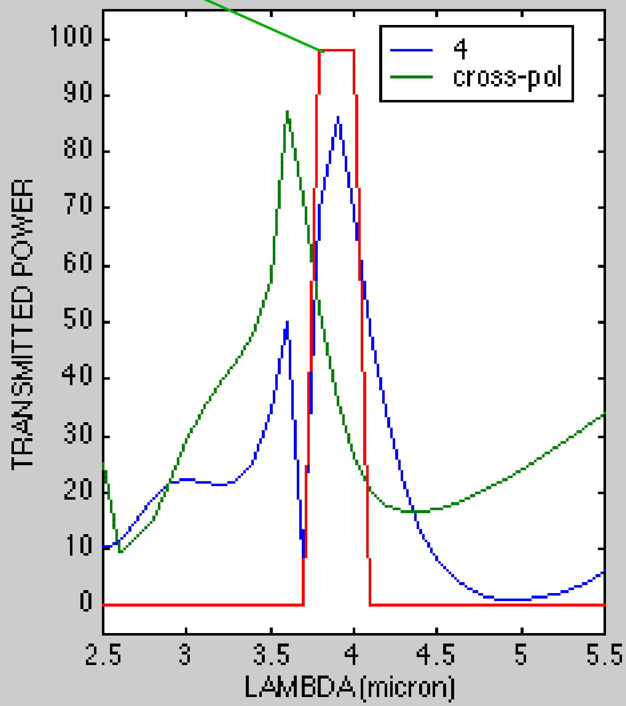


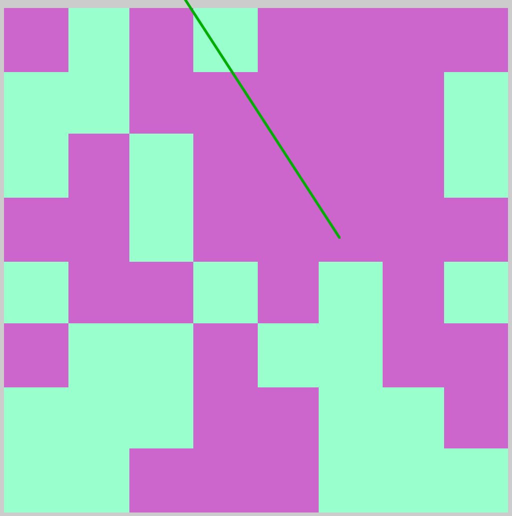


Optical Filter Design

Maximize linear polarization response to **prescribed response**
Minimize opposite and cross polarizations

16x16 pixels
Mettalization
No Metal





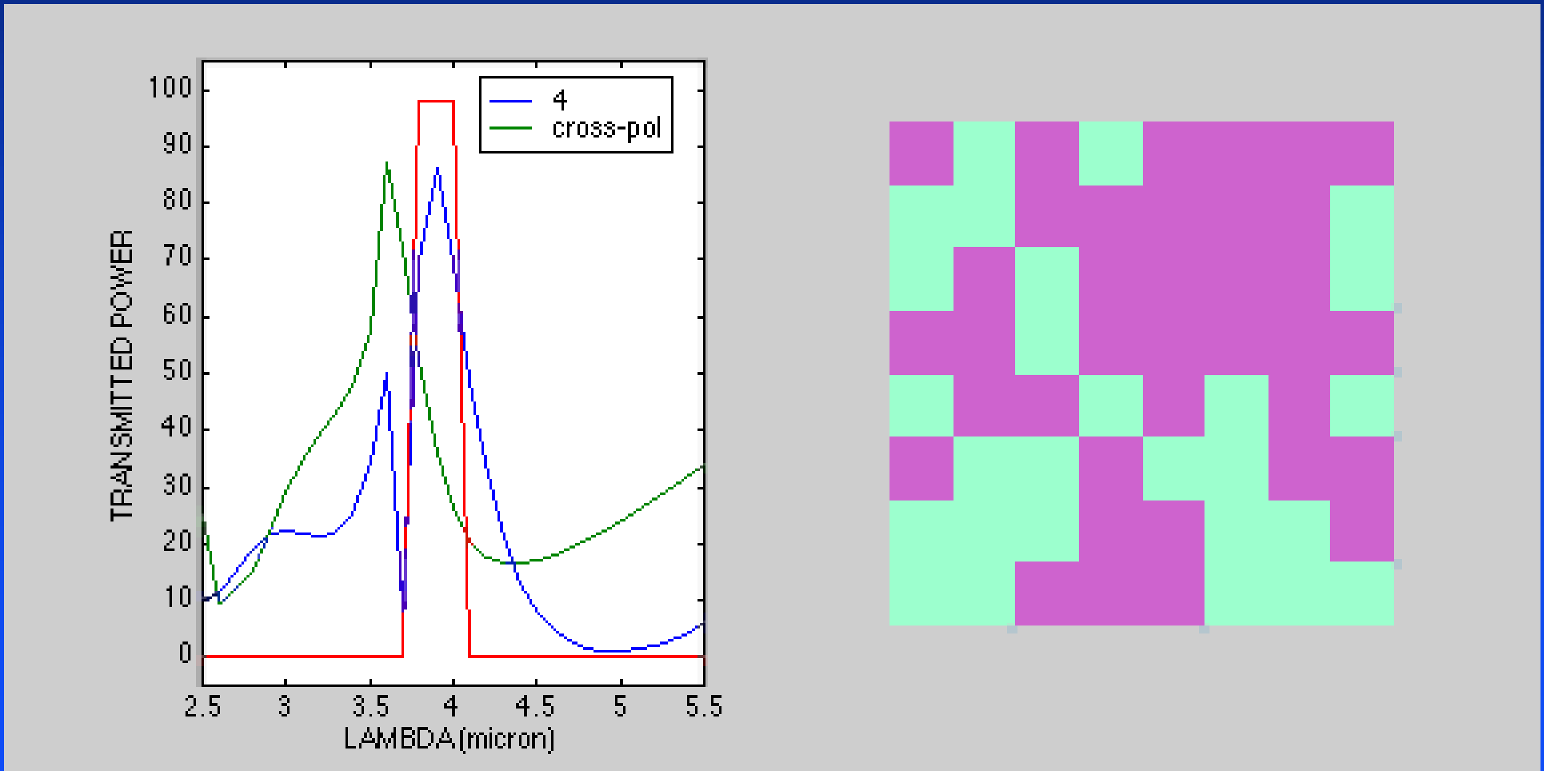
Genetic Algorithm Design Evolution

Optimization of Slot Array

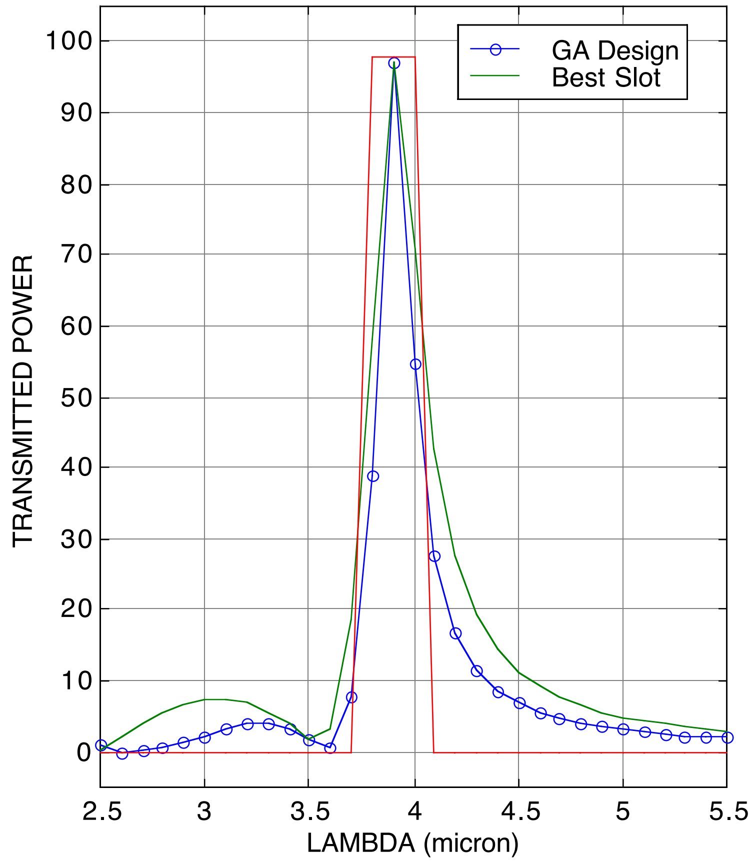
pop = 630, 300 generations, steady-state (10%), 2-point crossover p = 0.85, mutatation p = 1/64

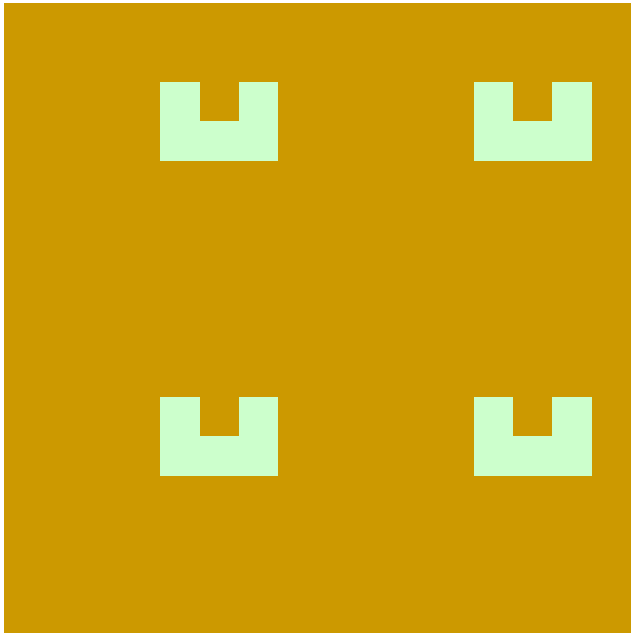
=> 19,467~$2x10^5$

Exhaustive Search: $2^{64} \sim 1.8x10^{19}$



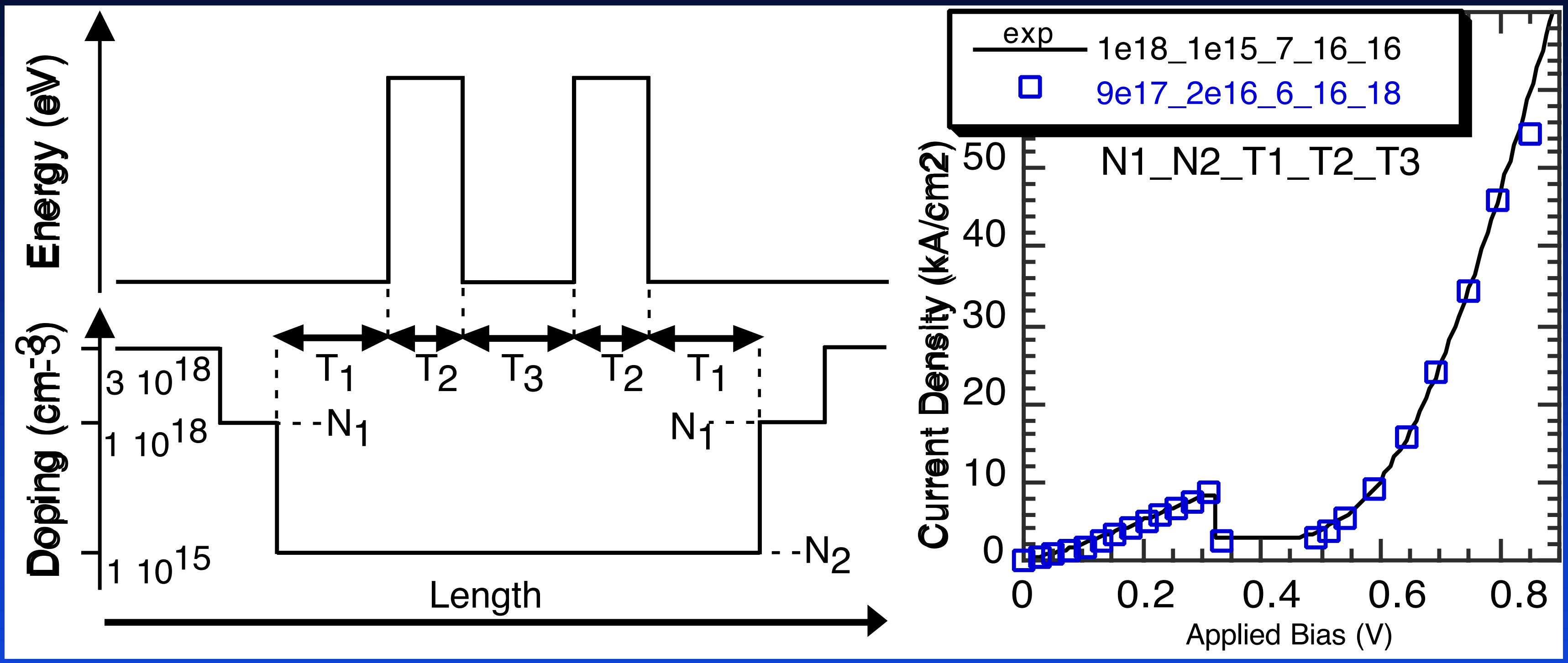
Genetic Algorithm Design and Best Slot Array





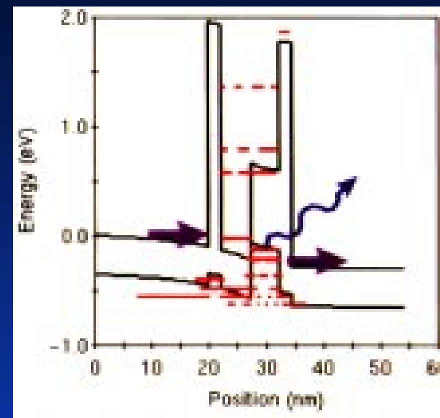
2x2 Portion of Array Design

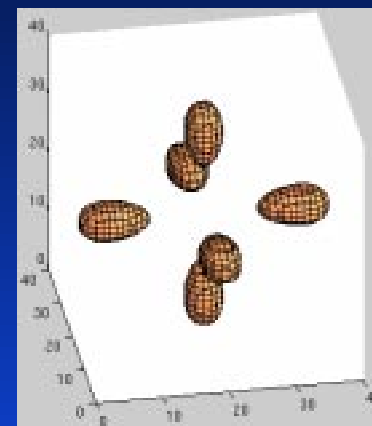
GENES - RTD Structural Analysis

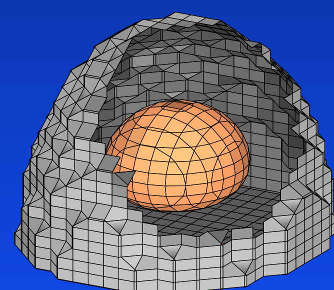


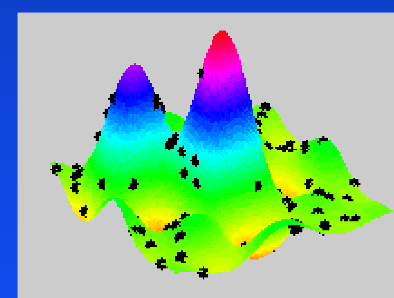
Future Efforts

- **1D:**
  - AC and optical interactions
  - Strain
  - Bandstructure (sp3d5)
  - Sb-based materials
- **3D:**
  - Strain
  - Bandstructure
  - Scattering
  - Coupled dot arrays
  - Open Dot Systems
- **Analysis & Synthesis**
  - Generalize optimization interface:
    - User input
    - Data output
    - Other algorithms





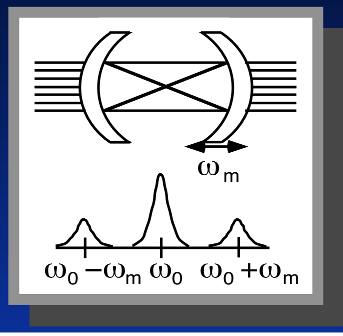




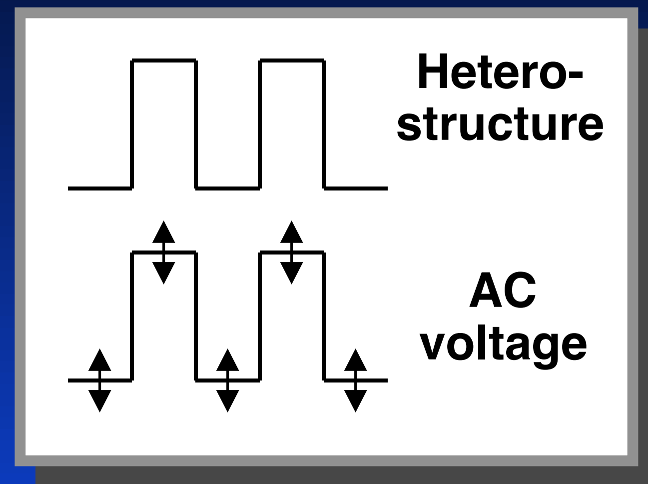
THz device technology
Detectors
Lasers

AC Simulation - Electron-Photon Interactions

Coupled Resonators



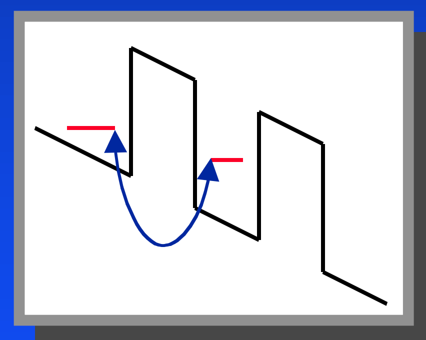
$$V_{ep} = \frac{1}{\sqrt{V}} \sum_{q} U_{\vec{q}} e^{i\vec{q}\bullet\vec{r}} \left(a_{\vec{q}} + a^{+}_{-\vec{q}} \right)$$



Electron-Phonon & Electron-Photon interaction potentials are isomorphic

Future NEMO capabilities:

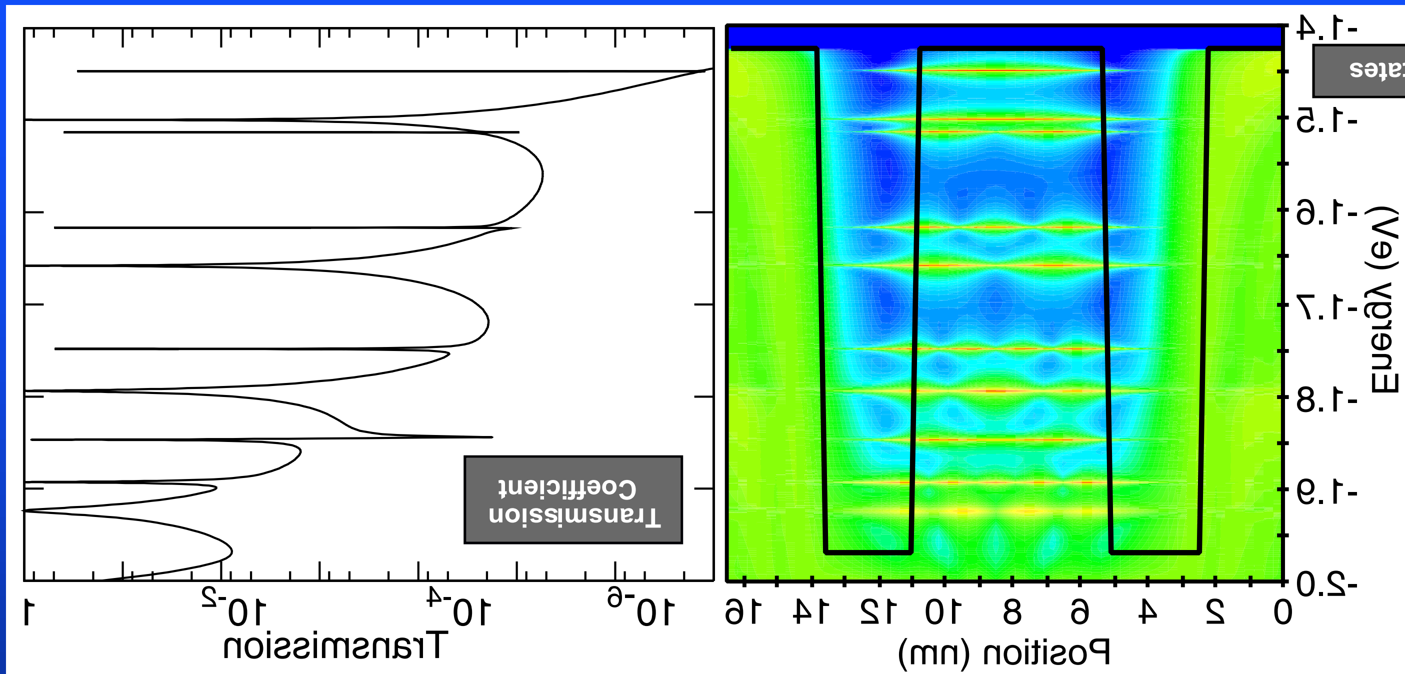
- **small signal AC response, one sideband, treatment via perturbation**
- **large signal response, multiple sidebands, non-perturbative treatment**



Caveat:
Realistic RTD's are Always coupled quantum wells

Interesting problem:
Charge oscillations between the wells

Steps towards Laser Modeling: Heterostructure Hole Transport



Approach:
- Use real space tight binding bandstructure representation to resolve finite size of heterostructures. (nearest and second nearest neighbor sp3s*)
- Examine dependence on transverse momentum and resonance broadening.

Objective:
- Long Term: Develop ability to model electron and hole interactions in a semiconductor laser including transport.
- Short Term: Analyze transport in a hole resonant tunneling diode.

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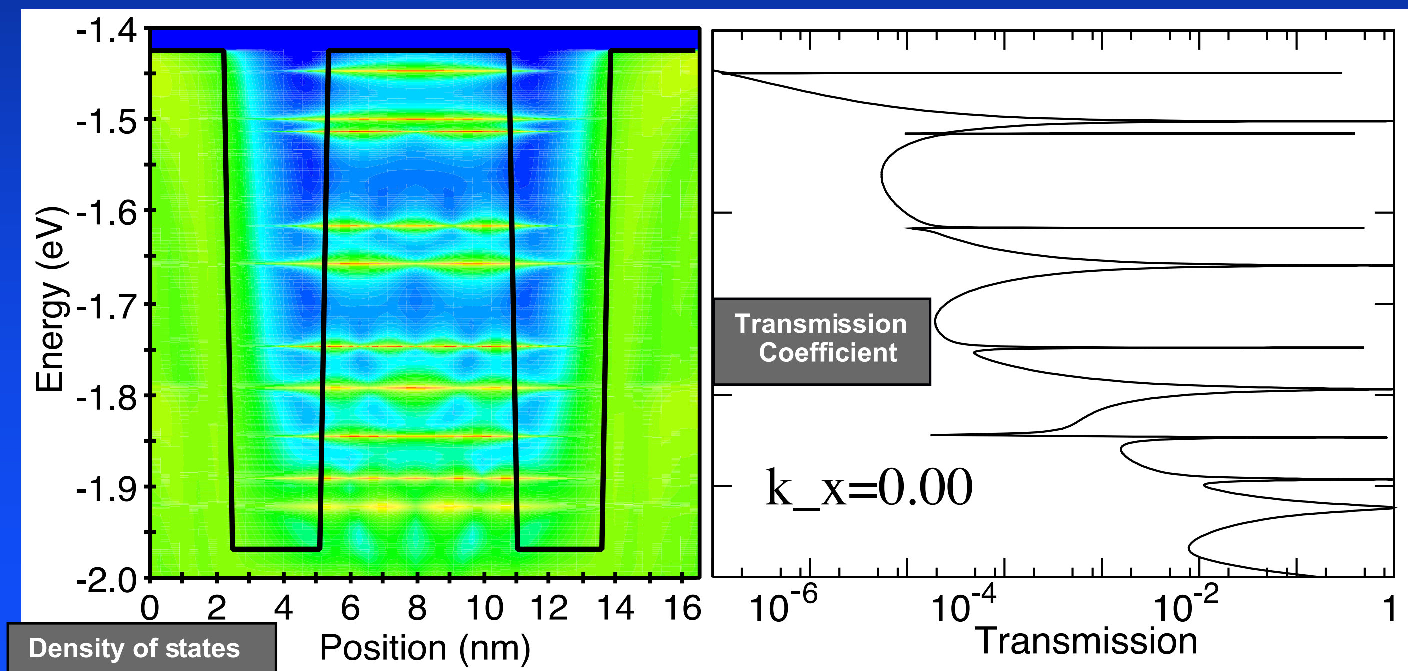

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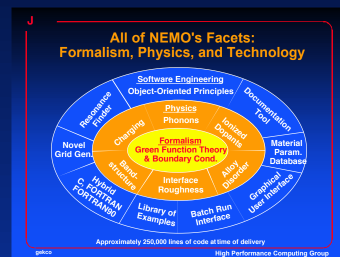
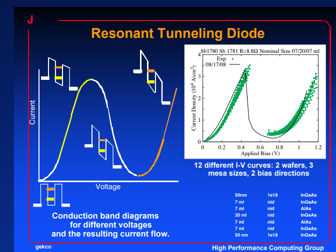
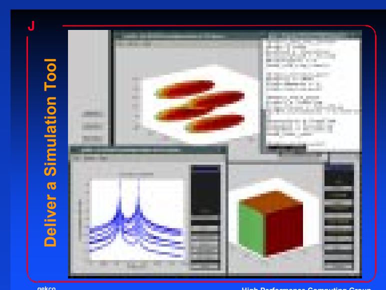
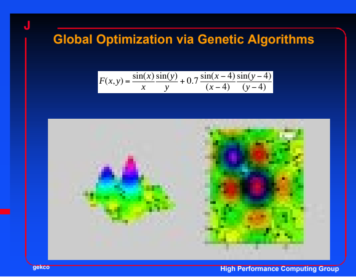
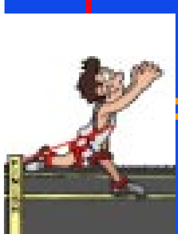


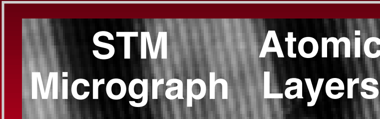




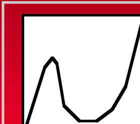




Atomic scale physics



Practical devices



Macroscopic currents and radiation

Systems on a chip

Any Questions?